*Fig. 1*

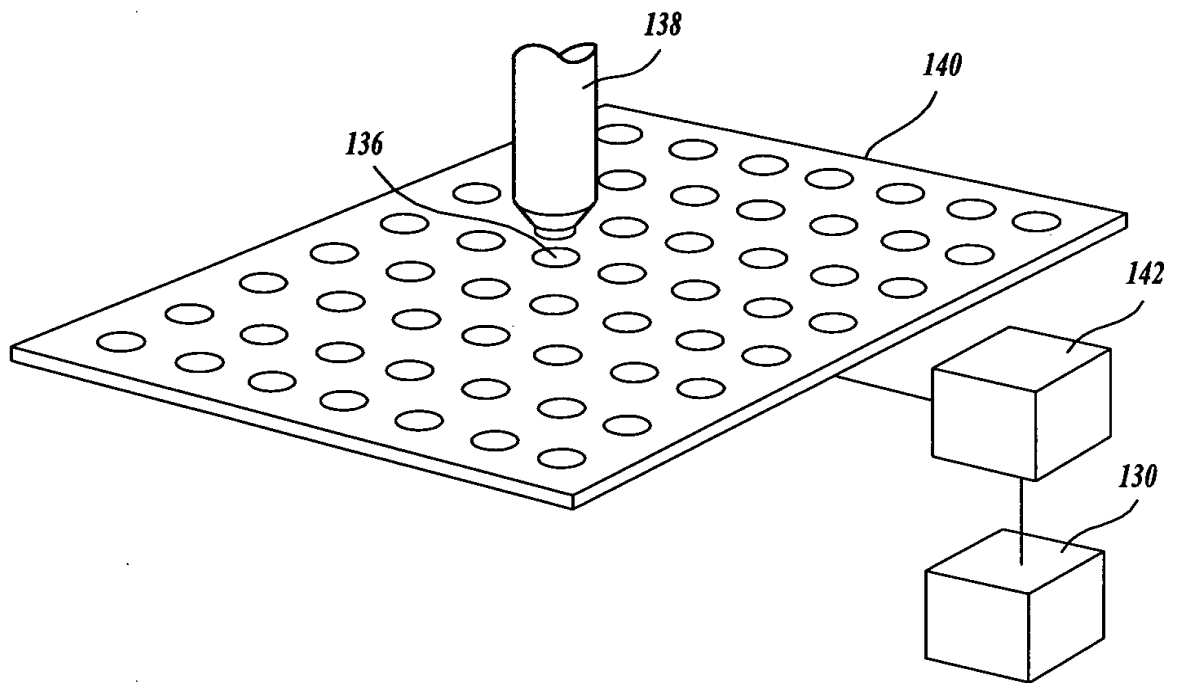


Fig. 1A

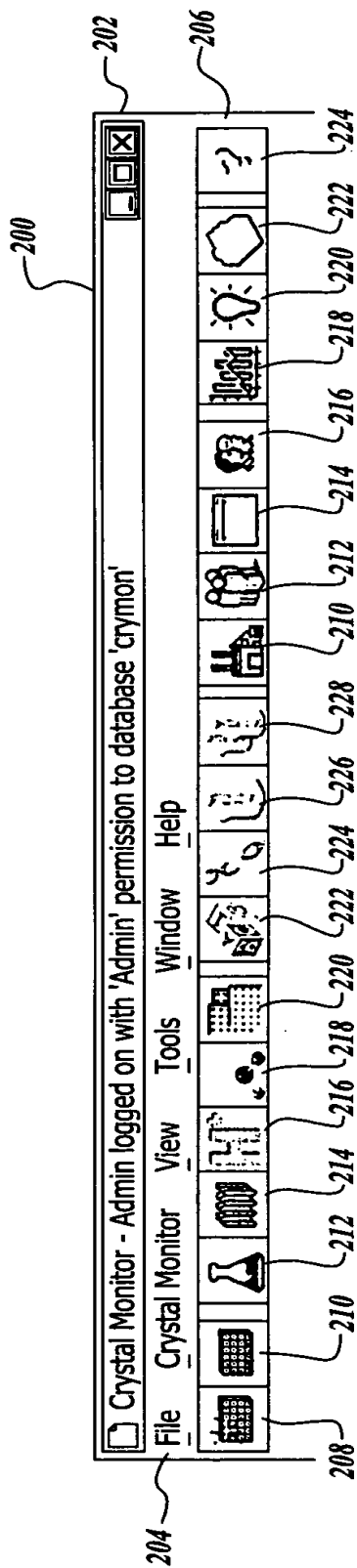
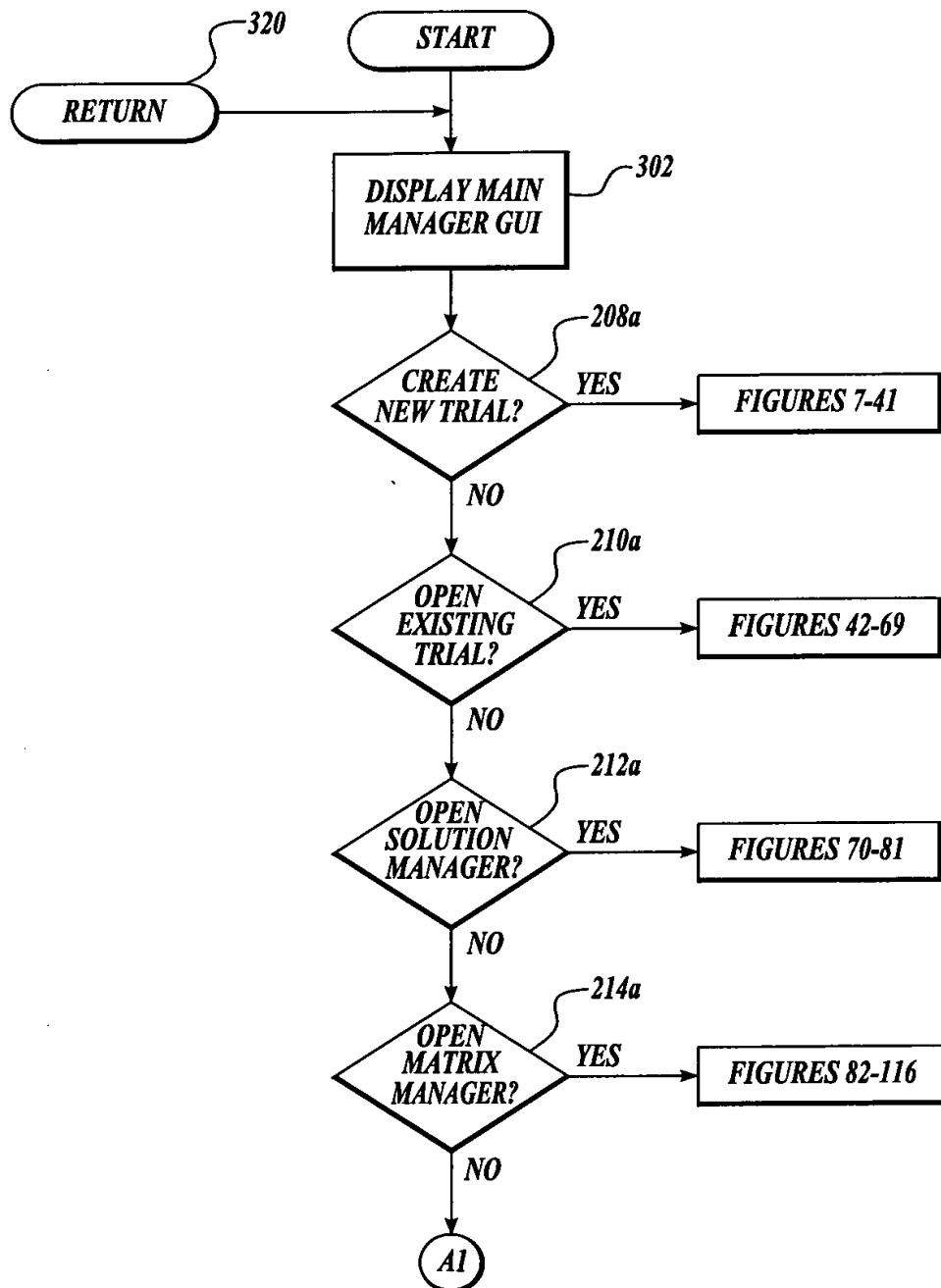


Fig. 2

*Fig. 3*

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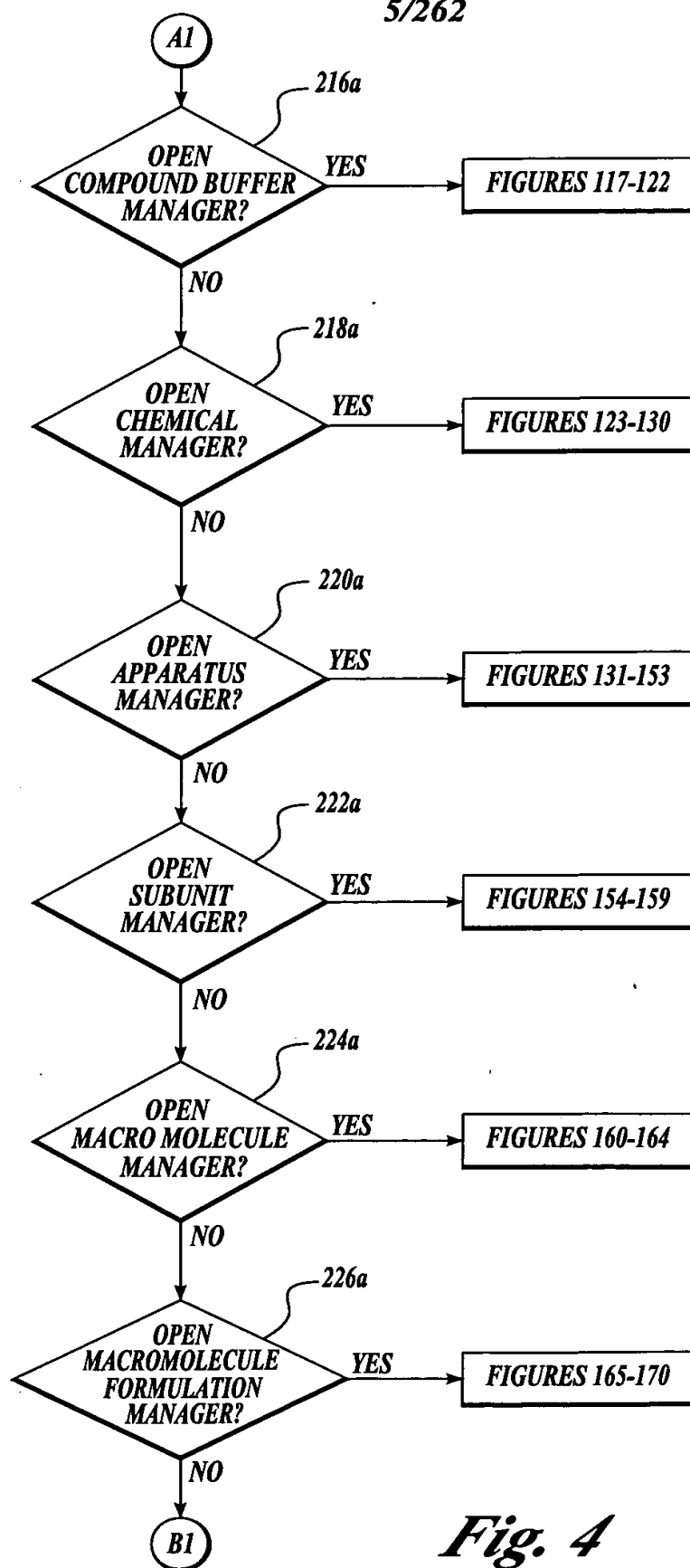
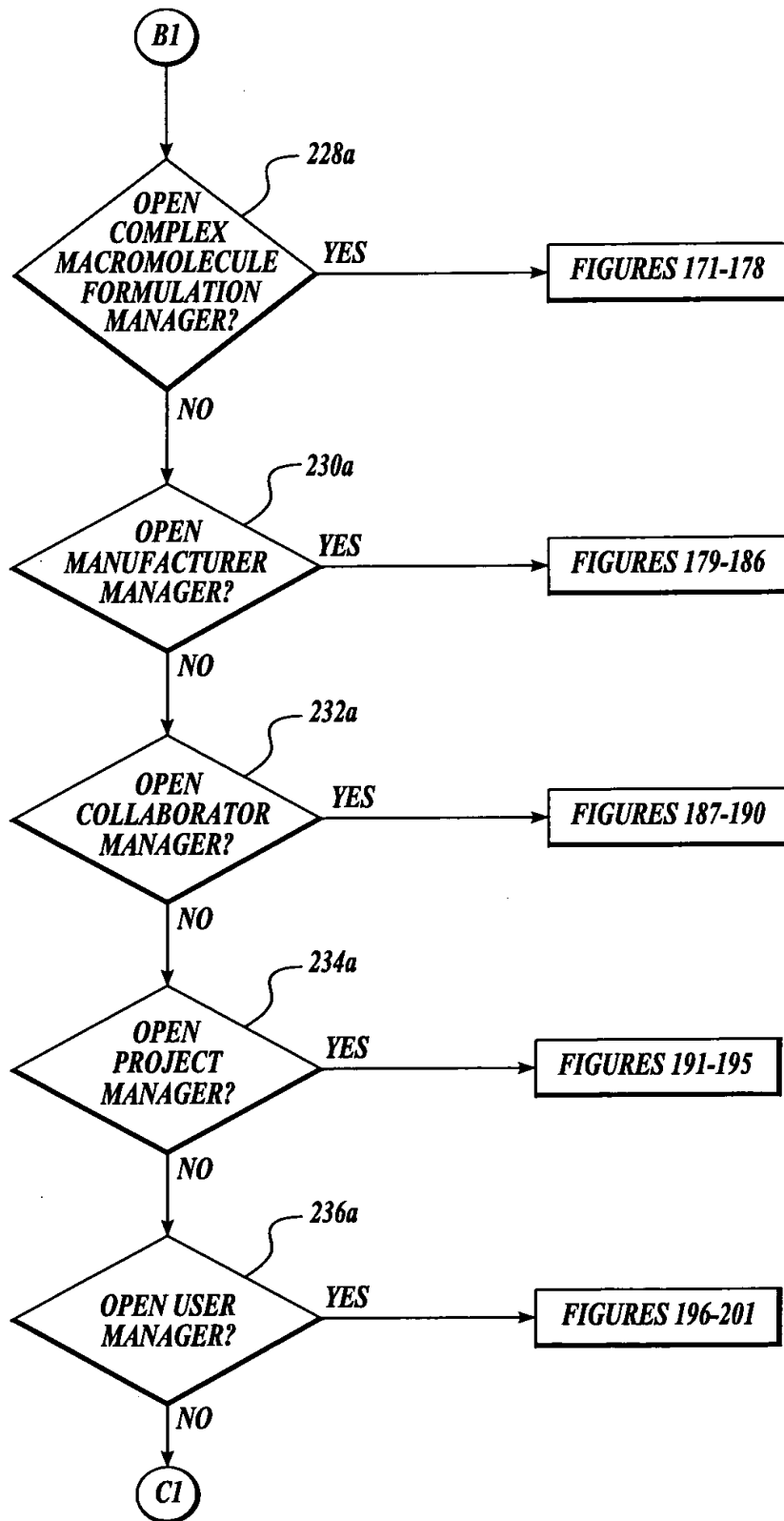
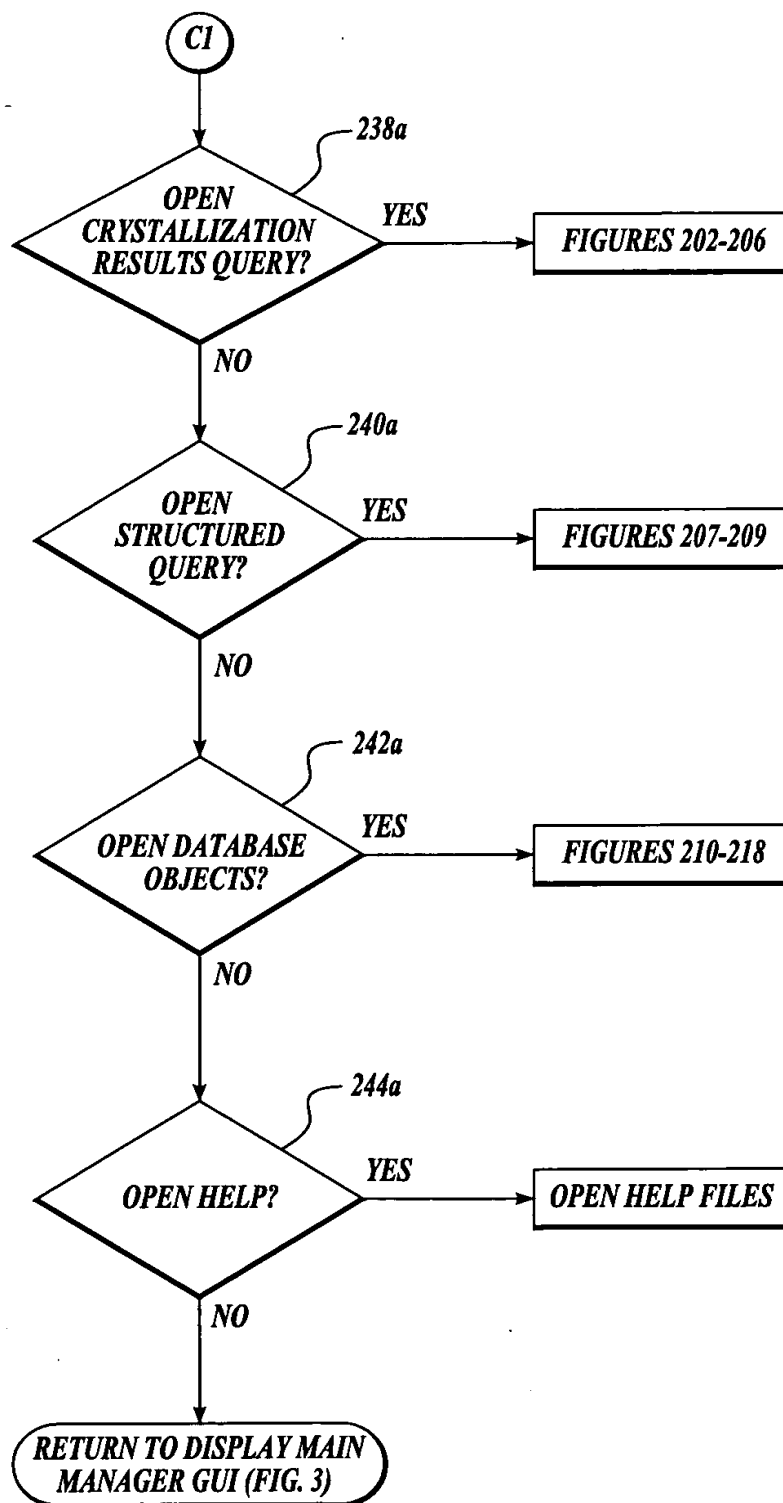


Fig. 4

*Fig. 5*

*Fig. 6*

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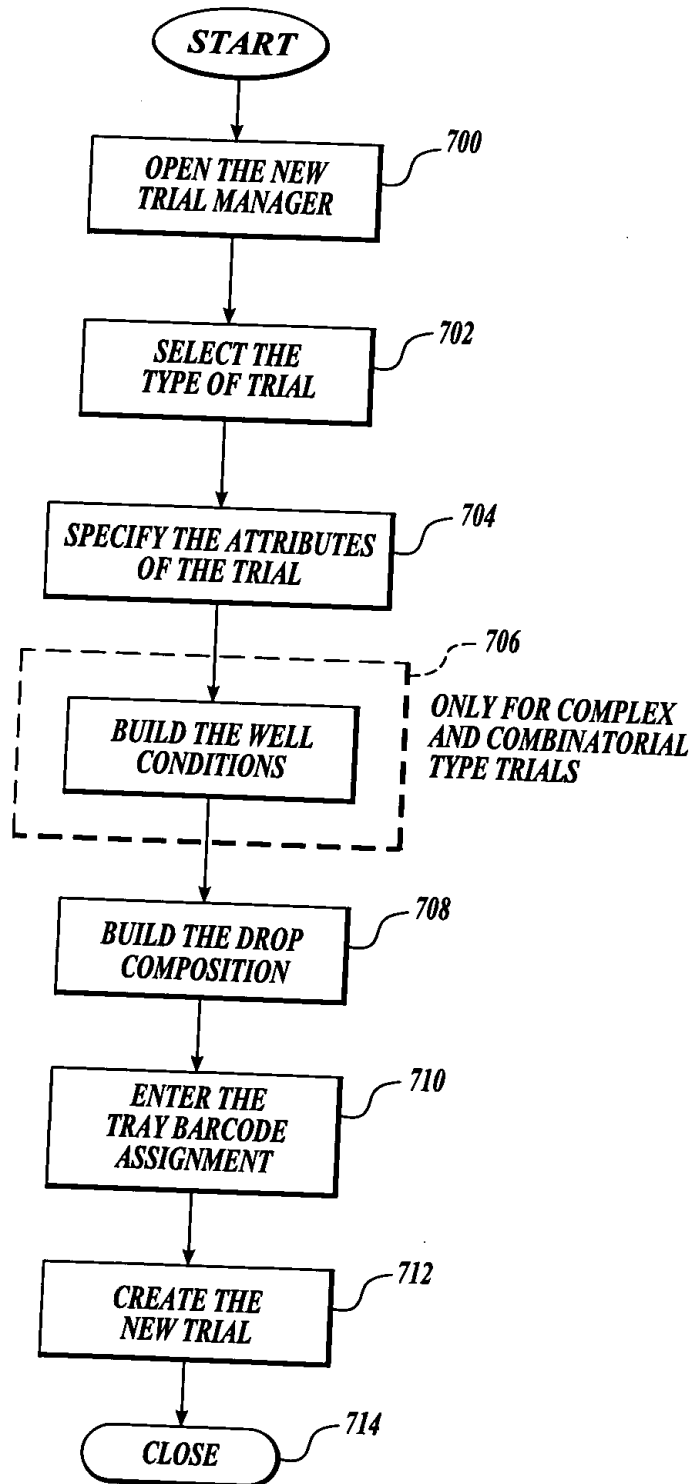
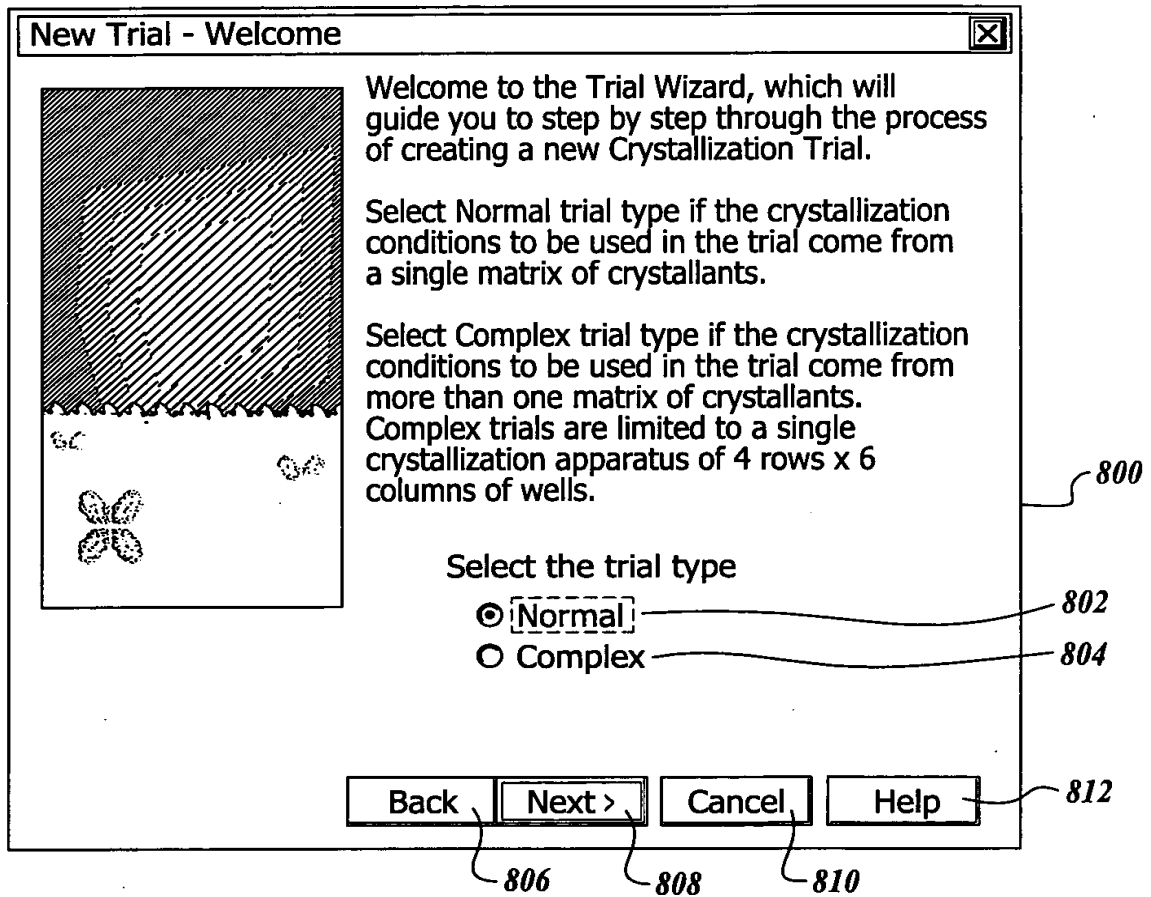
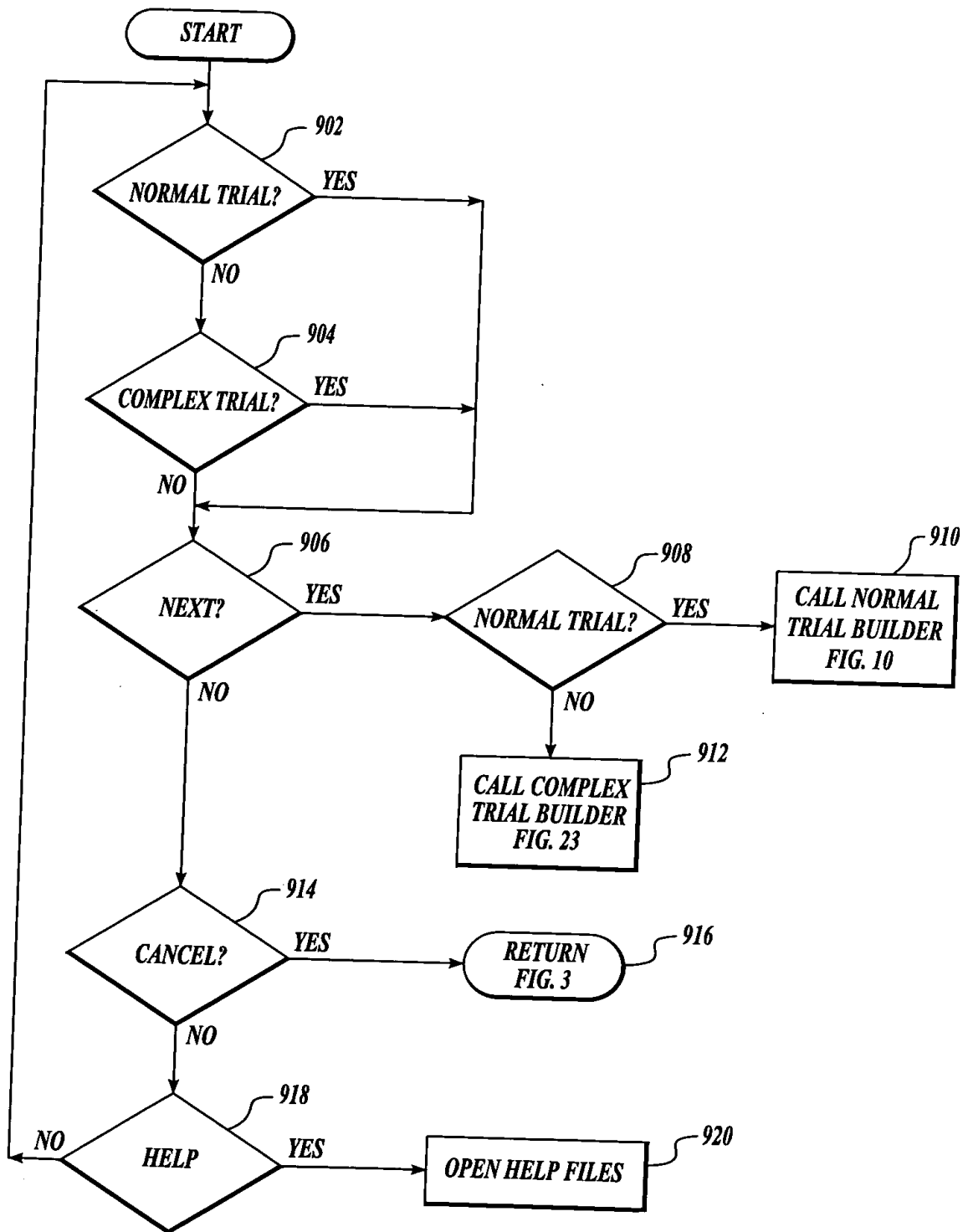


Fig. 7

*Fig. 8*

*Fig. 9*

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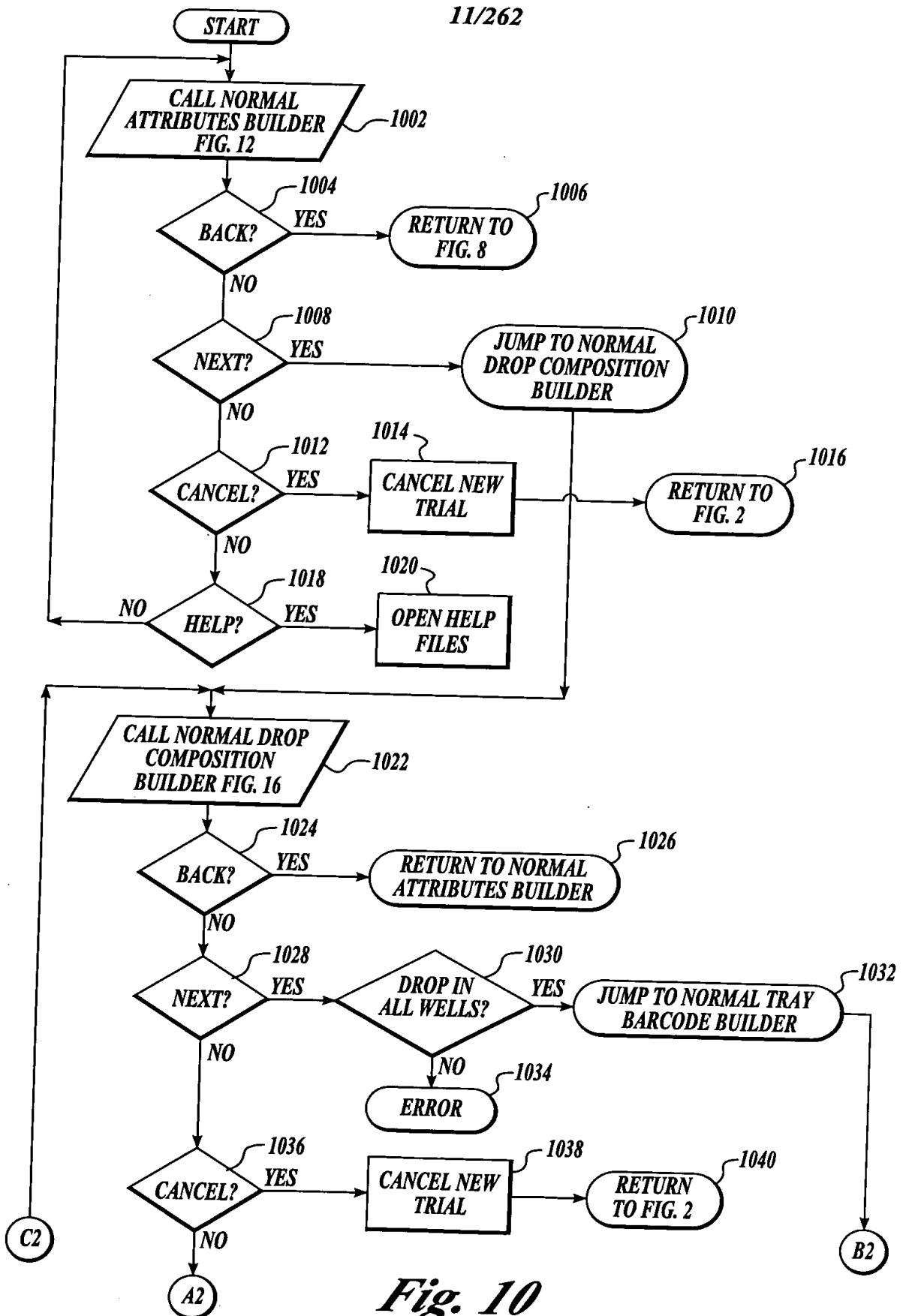
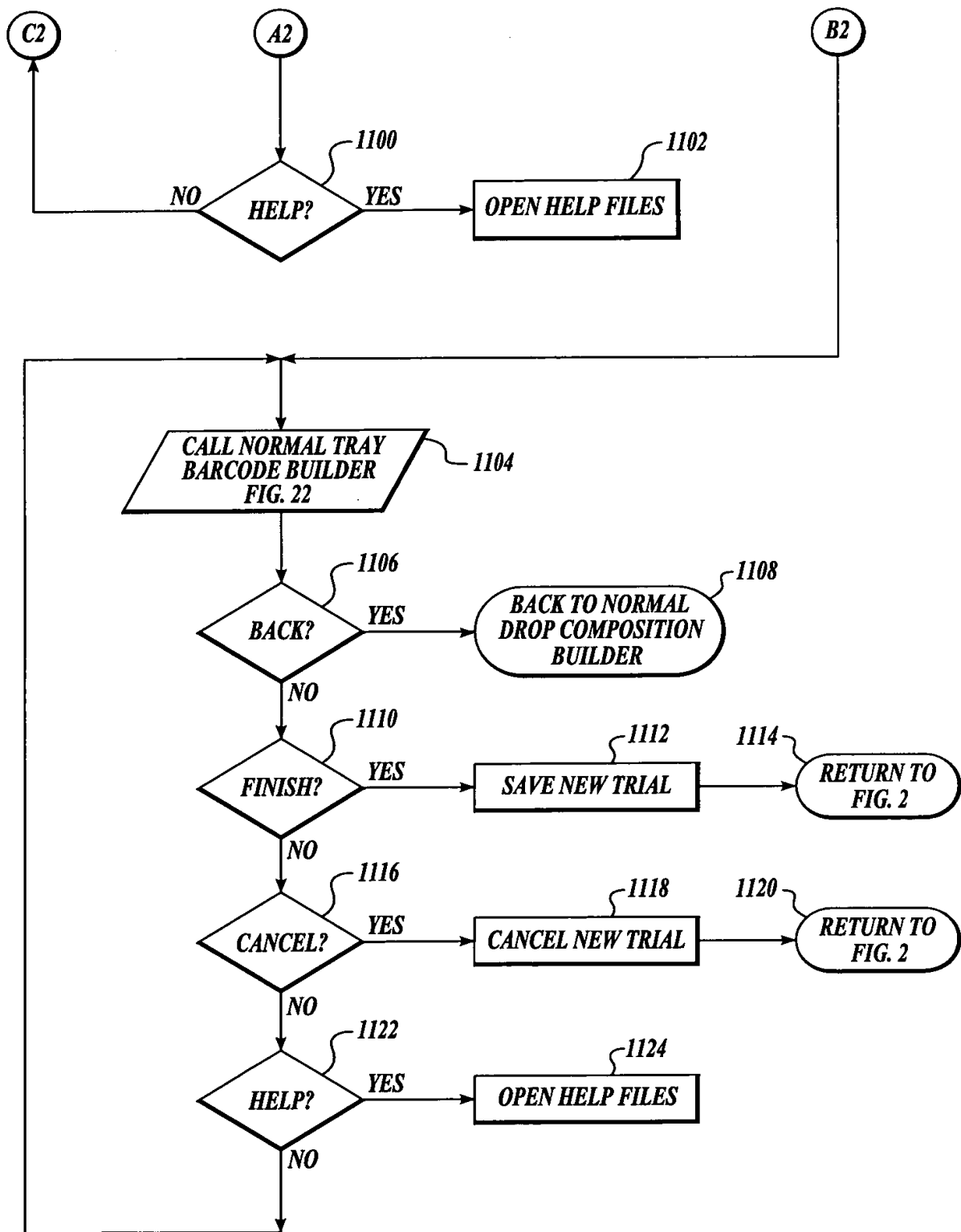


Fig. 10

*Fig. 11*

New Trial - Specify Attributes

Project: jjprotein
 Collaborator: Emerald BioStructures
 Apparatus: Charles Supper Plate
 Gas Purge: <None>
 Temperature: 25. C
 Reservoir Volume: 200 µl
 Prep. Date: 4/ 3/00

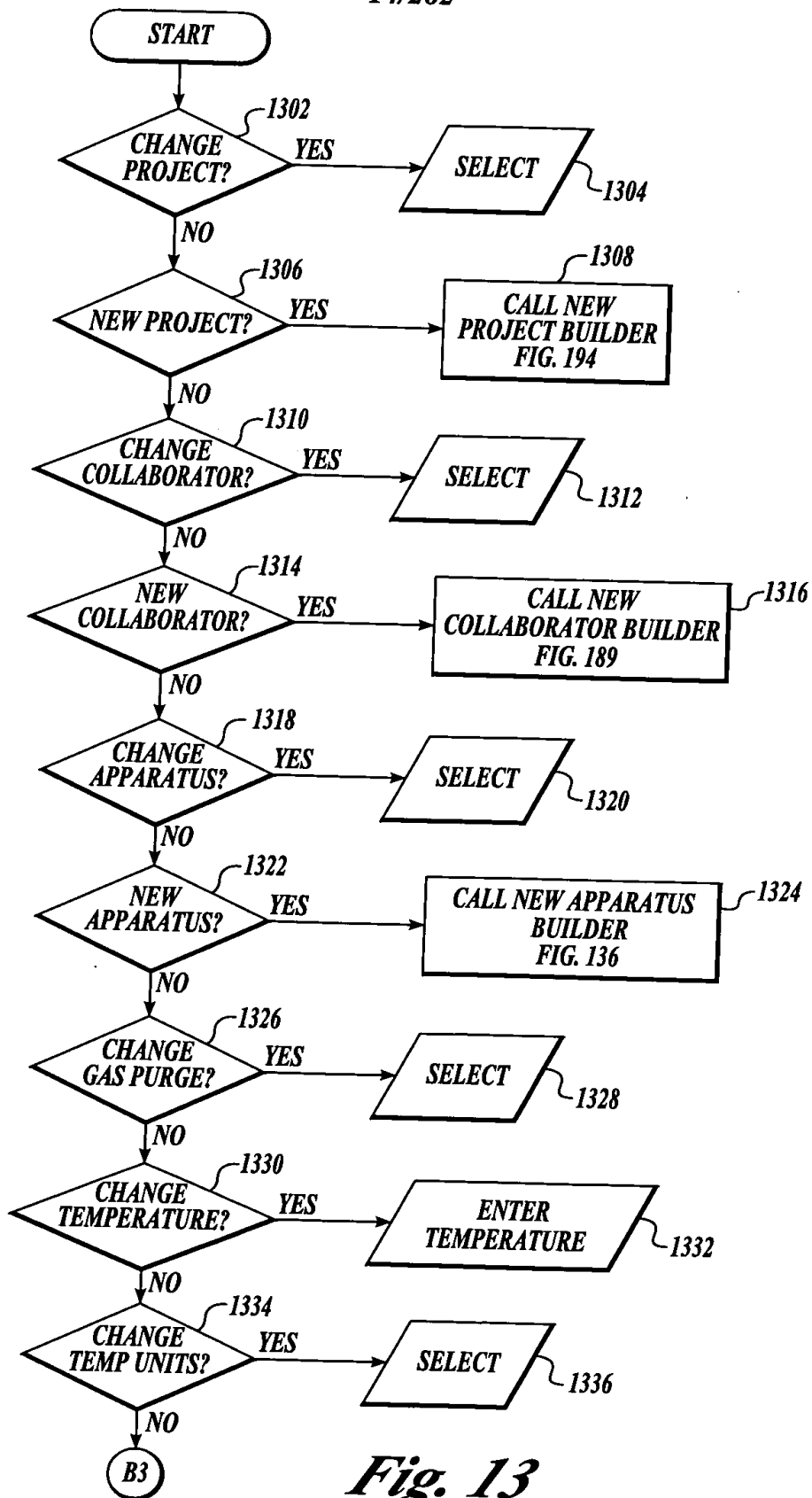
Matrix: Wzrd1

Oil Overlay: <None>
 Oil Overlay Volume: 1258

Buttons: Back, Next >, Cancel, Help

Figure 12 is a screenshot of a software dialog box titled "New Trial - Specify Attributes". The dialog box contains several input fields and buttons. On the left, there is a preview window showing a complex, branching, fractal-like structure. The main area contains the following fields: "Project" (jjprotein), "Collaborator" (Emerald BioStructures), "Apparatus" (Charles Supper Plate), "Gas Purge" (<None>), "Temperature" (25. C), "Reservoir Volume" (200 µl), and "Prep. Date" (4/ 3/00). Below these is a "Matrix" field with the value "Wzrd1". Further down is an "Oil Overlay" section with a dropdown menu set to "<None>" and an "Oil Overlay Volume" field with a value of 1258. At the bottom, there are four buttons: "Back", "Next >", "Cancel", and "Help". The dialog box has a standard Windows-style title bar and a close button in the top right corner.

Fig. 12

*Fig. 13*

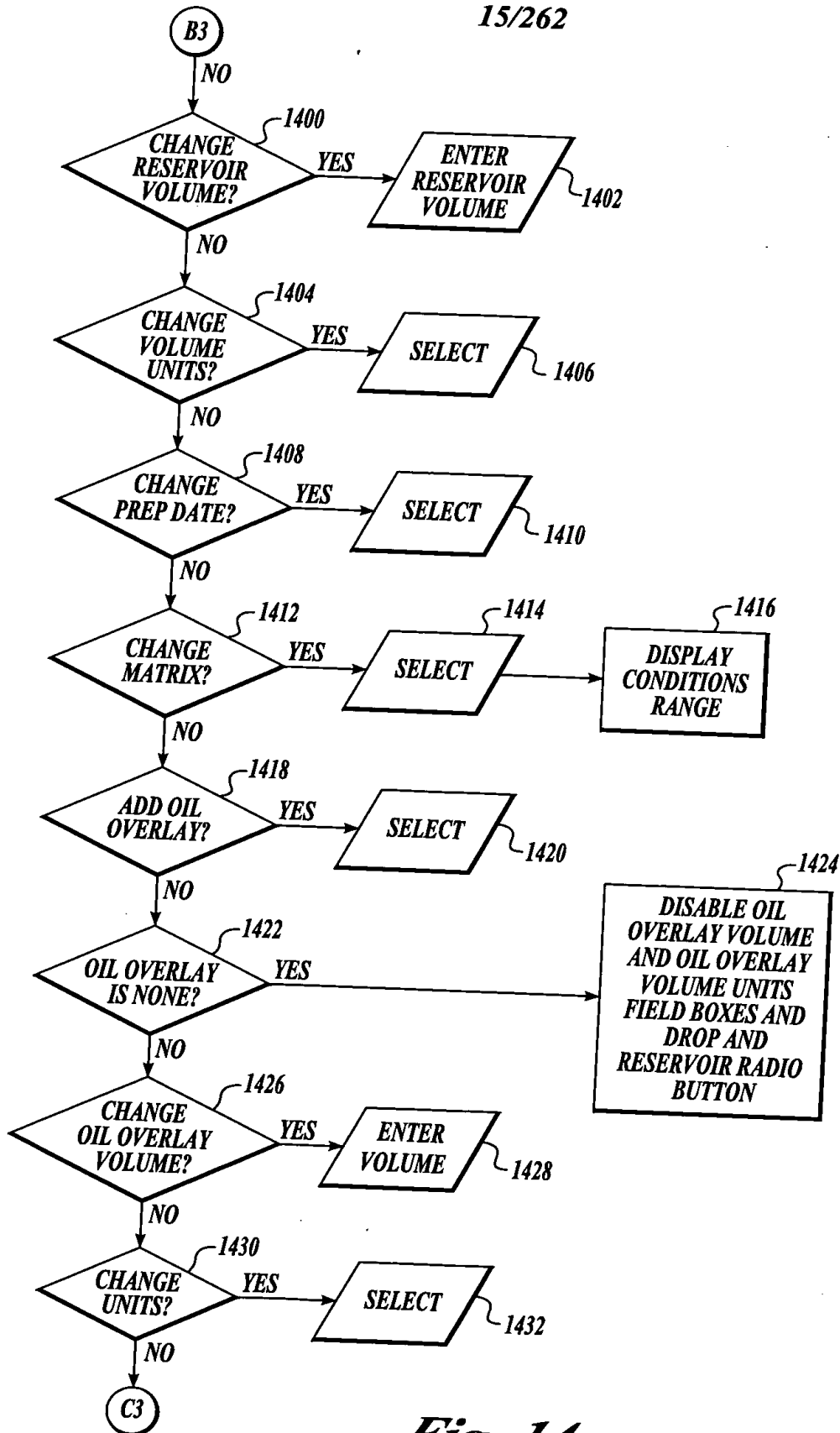
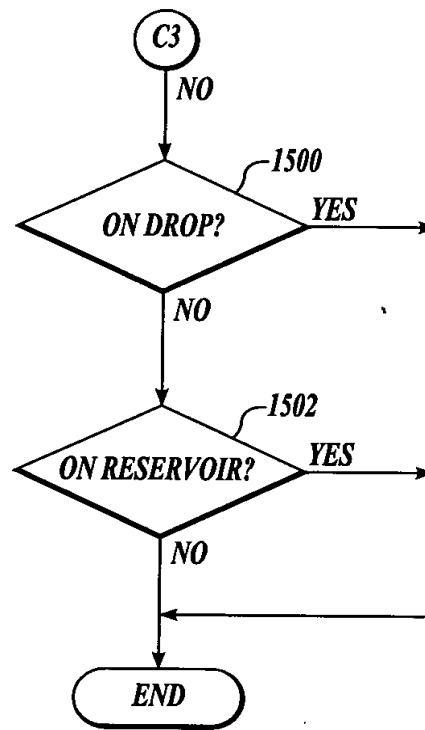
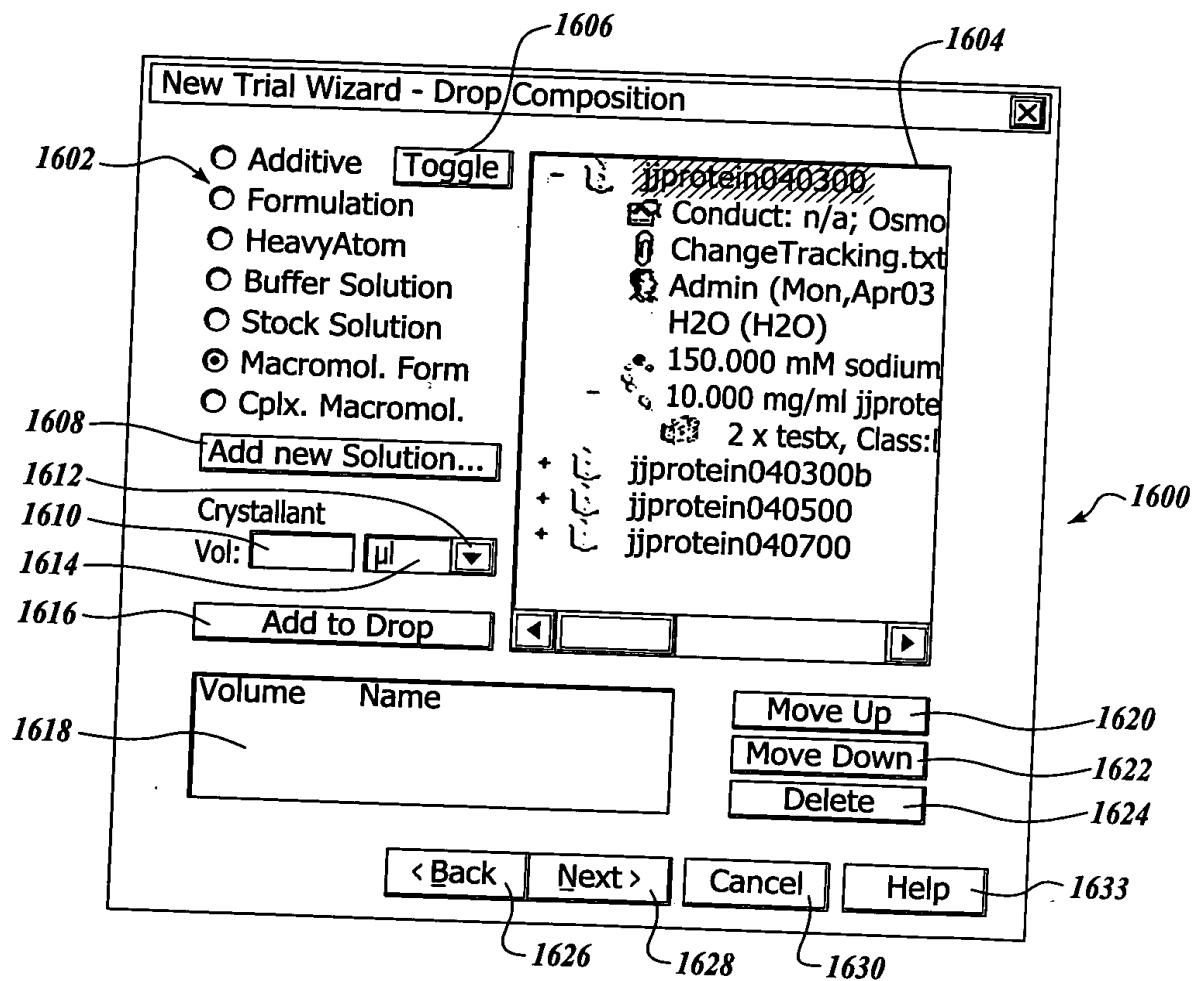
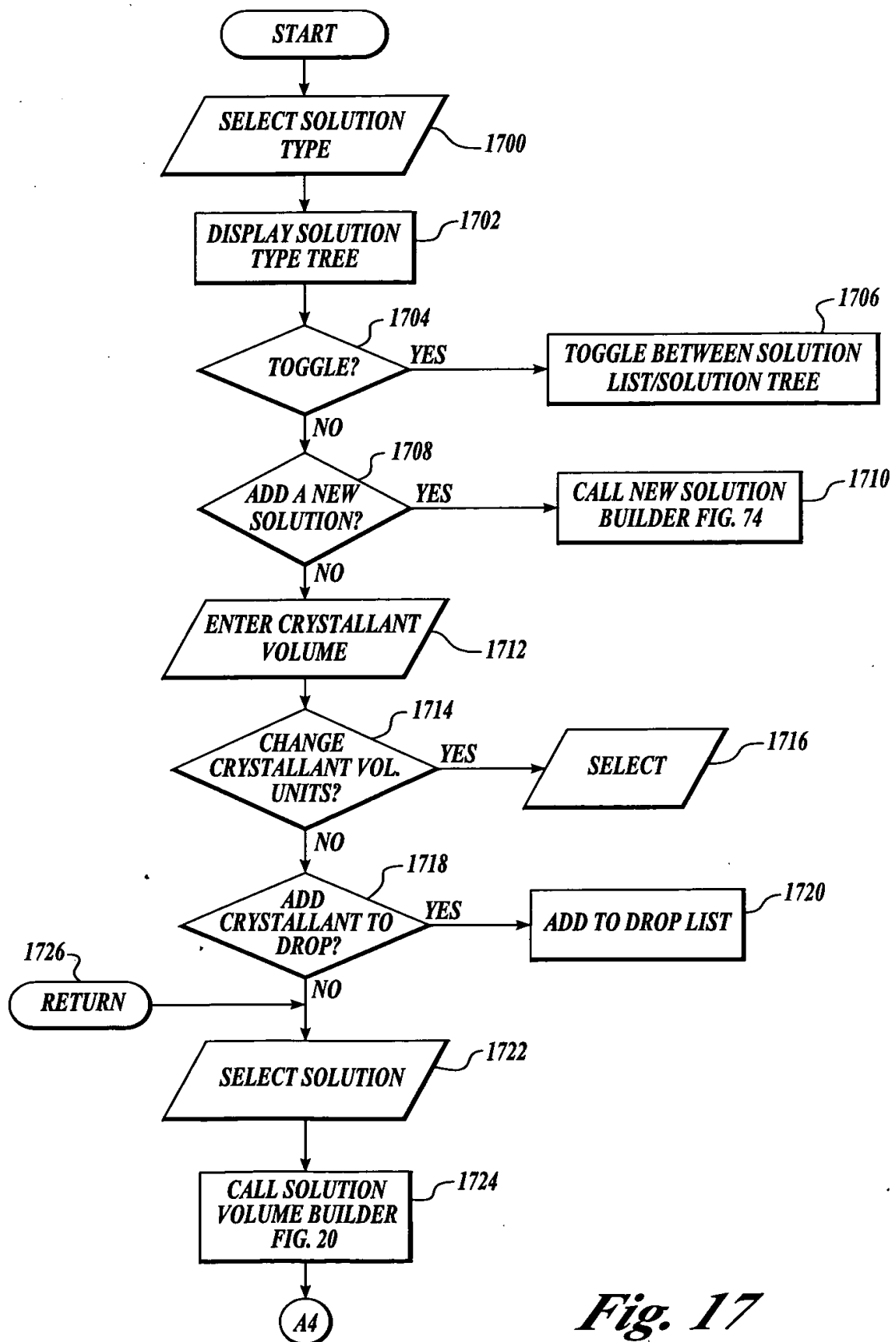
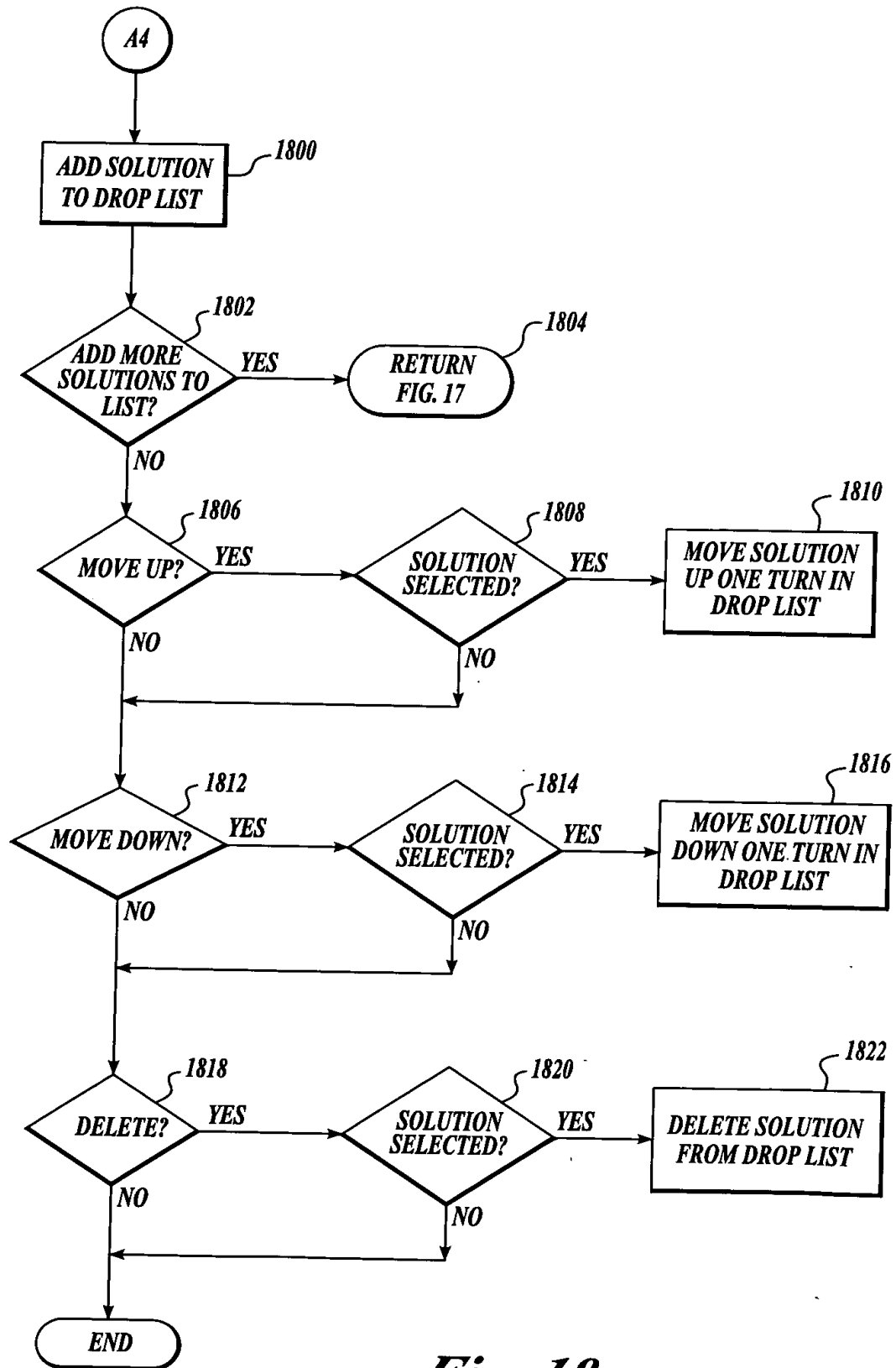


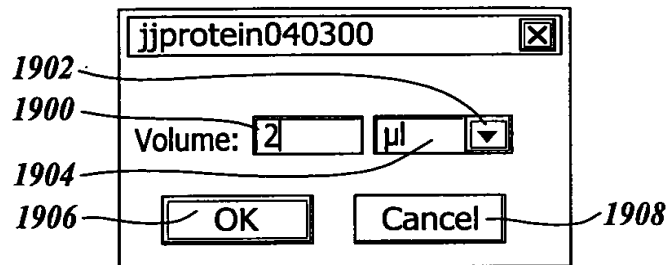
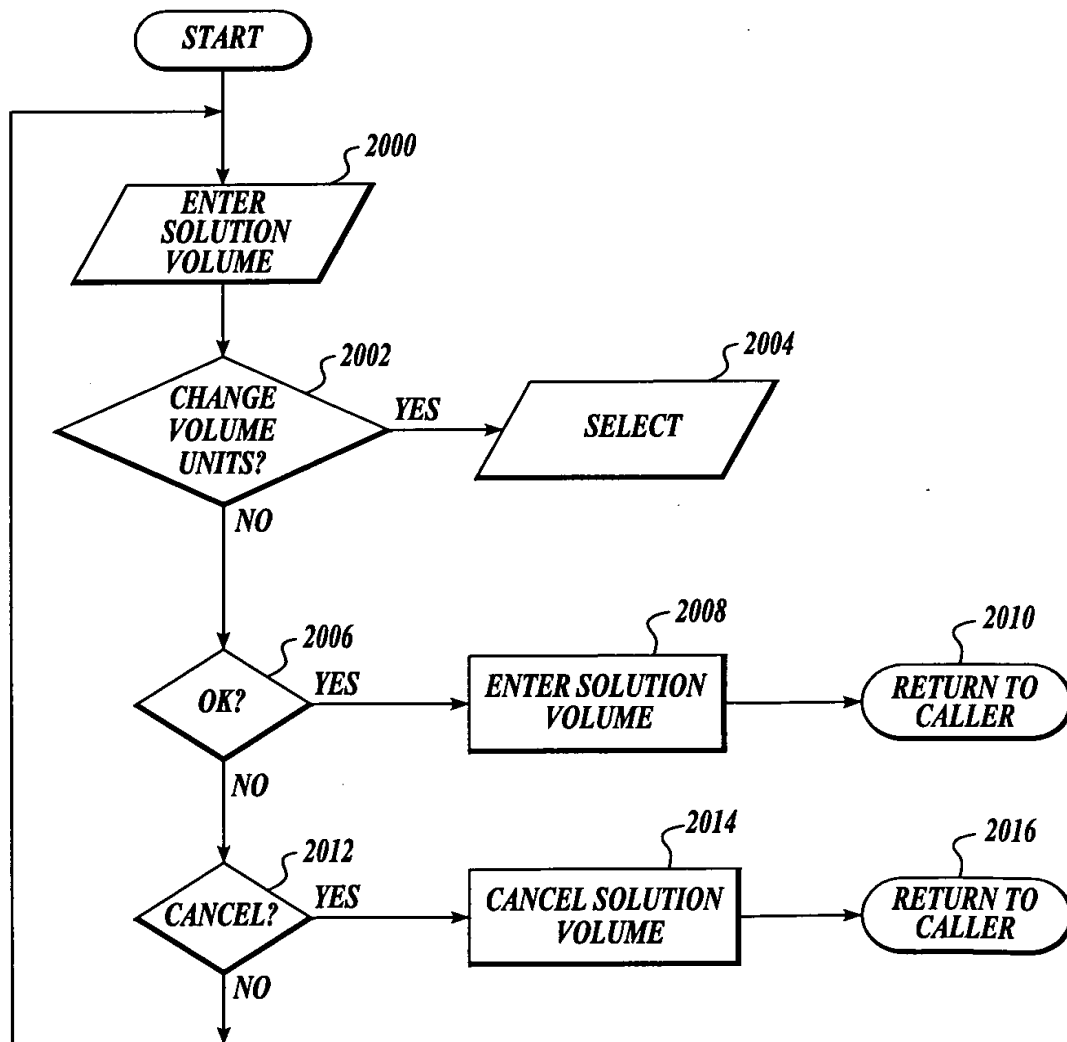
Fig. 14

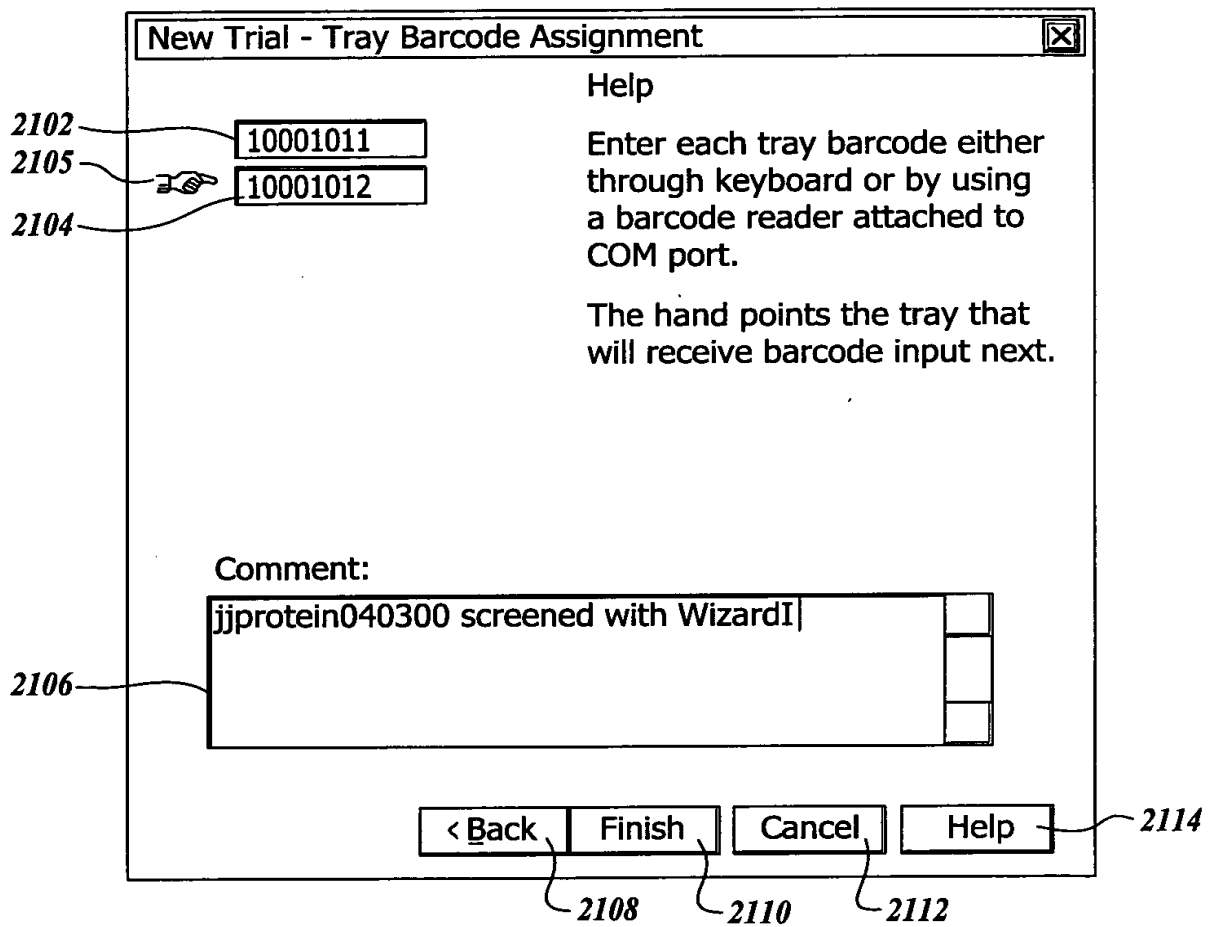
*Fig. 15*

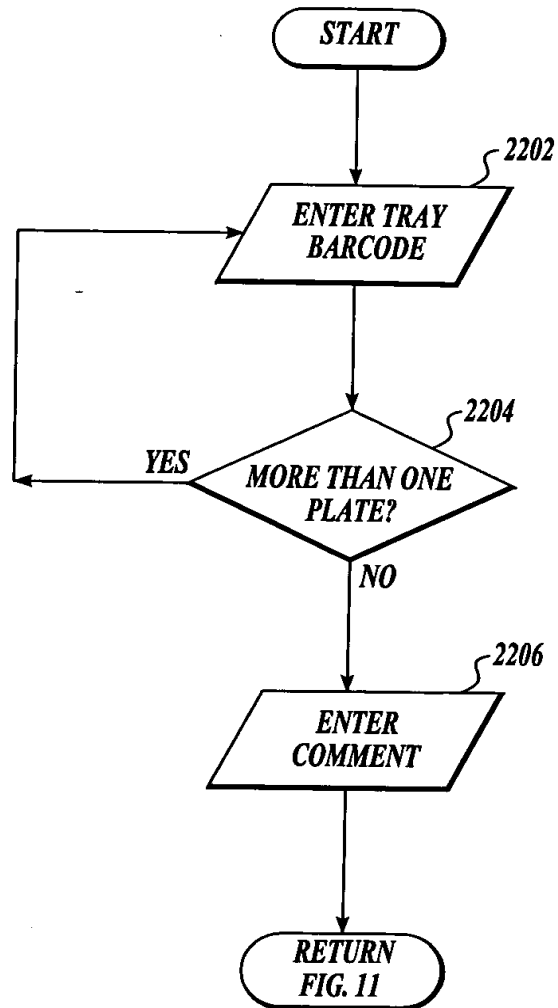
*Fig. 16*

*Fig. 17*

*Fig. 18*

*Fig. 19**Fig. 20*

*Fig. 21*

*Fig. 22*

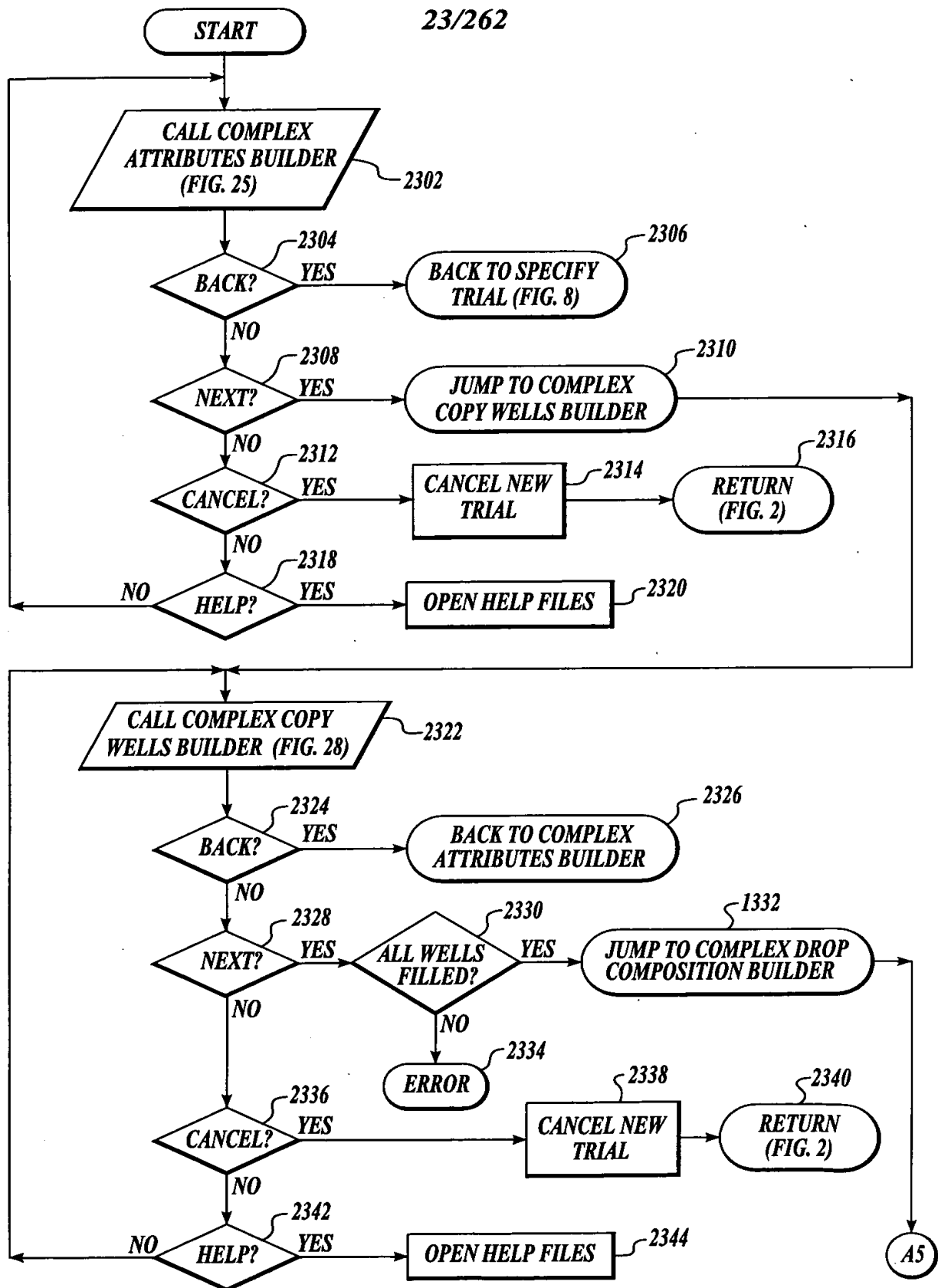


Fig. 23

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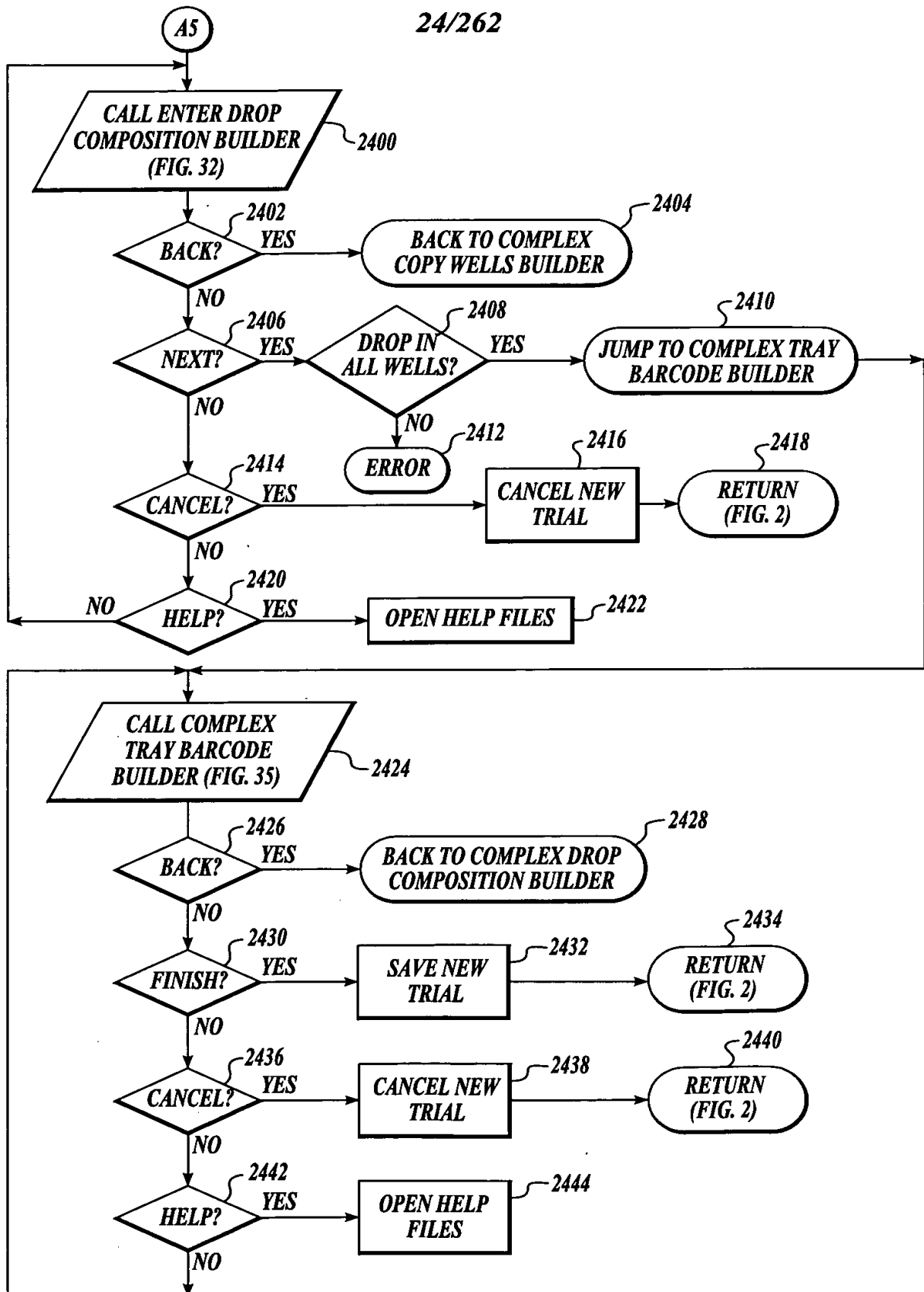


Fig. 24

2500

2520

2522

2501

2508

2502

New Trial - Specify Attributes

Project

Collaborator:

Apparatus:

Gas Purge:

Temperature:

Reservoir Volume:

Prep. Date: 2528

2536

2504

2510

2506

2516

2512

2514

2518

2524

2526

2530

2534

Oil Overlay

Oil Overlay:

Oil Overlay Volume:

2546

2550

2540

2538

2542

2544

2548

2558

Back

Next >

Cancel

Help

2552

2554

2556

Fig. 25

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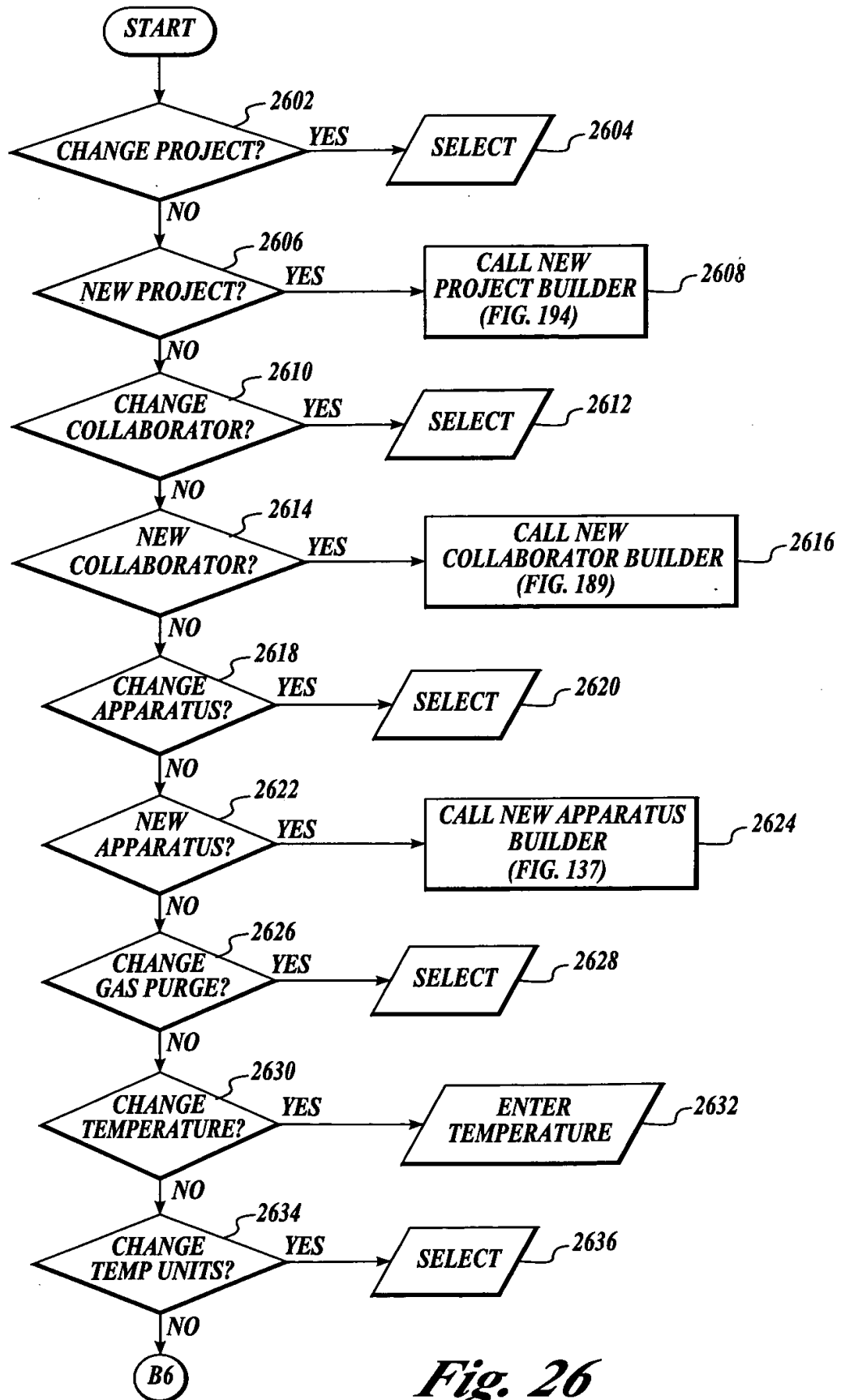


Fig. 26

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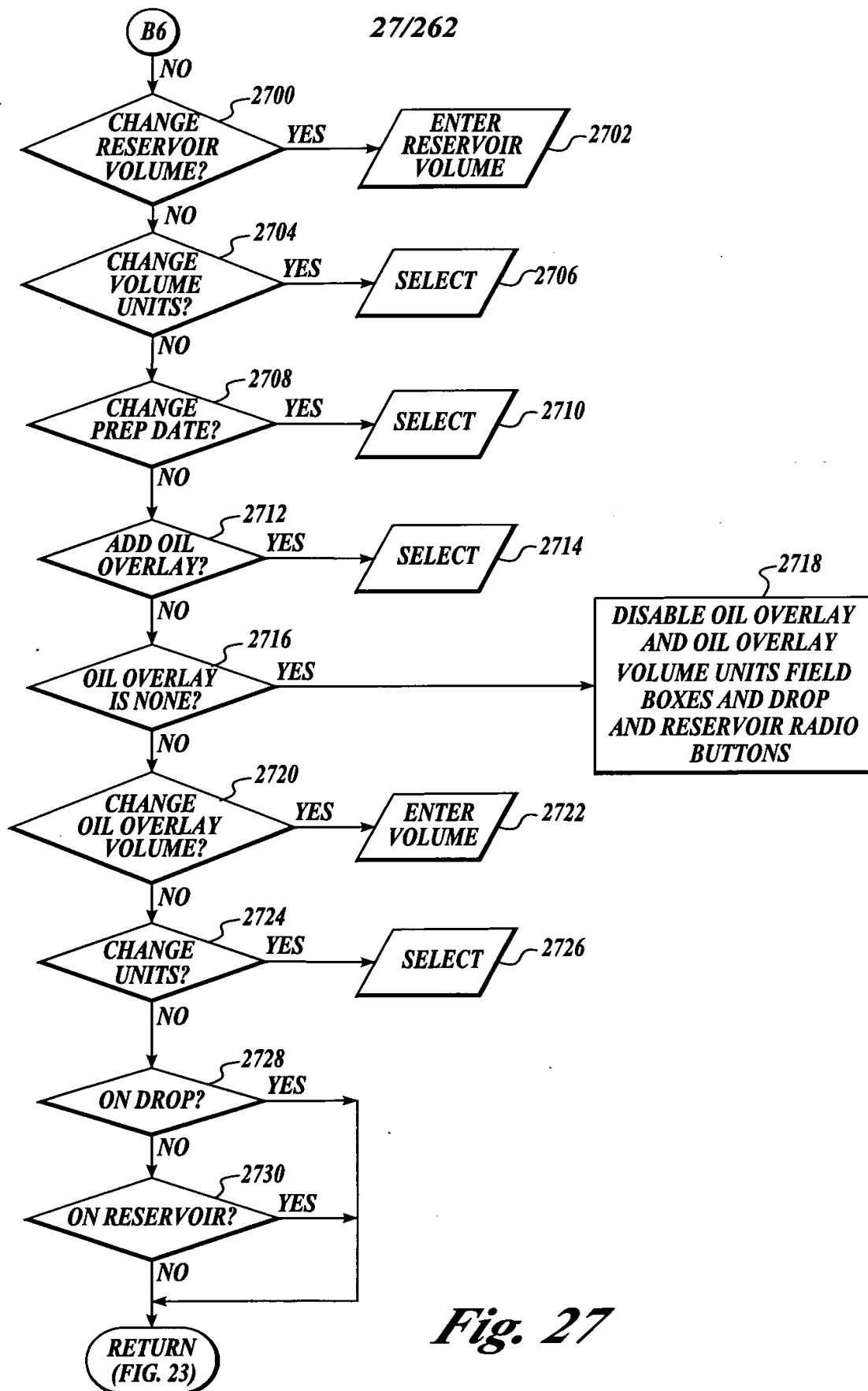
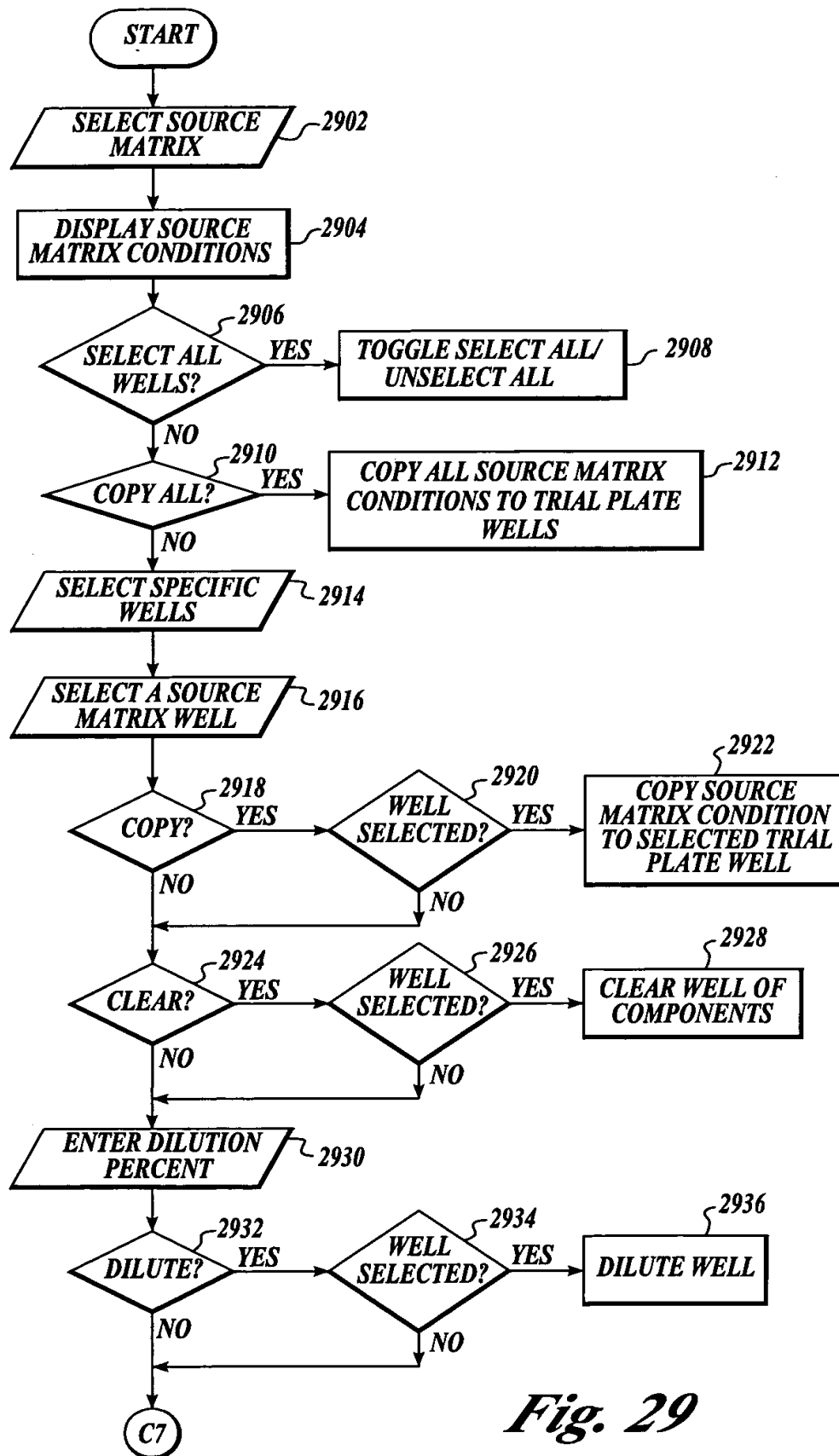
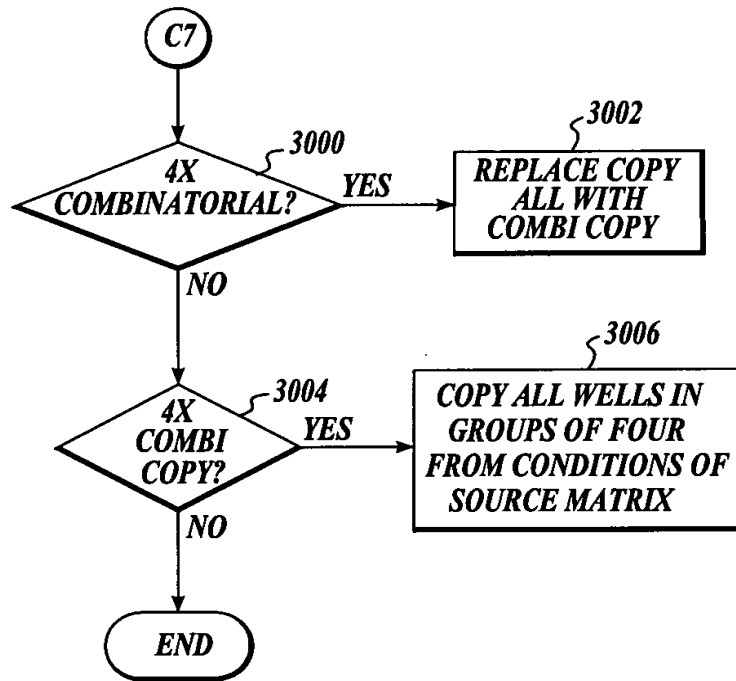


Fig. 27

*Fig. 29*

*Fig. 30*

3100 New Trial Wizard - Drop Composition

3101 ☐ Additive **3102** **List ->**

☐ Formulation

☐ HeavyAtom

☐ Buffer Solution

☐ Stock Solution

☒ Macromol. Form.

☐ Cplx. Macromol.

3103 + ☐ ijprotein040300
+ ☐ ijprotein040300b

3104 **Add new Solution...**

3106 Crystallant

3110 Vol:

3114

3112

Volume	Name
2.000 µl	ijprotein040300
2.000 µl	Crystallant

3128 **Transfer Drop to sel. Wells**

3126 **Clear Drop** **Sel all** **3124**

Charles Supper plate

(2) <input type="checkbox"/>	(2) <input type="checkbox"/>	(2) <input type="checkbox"/>	(2) <input type="checkbox"/>	(2) <input type="checkbox"/>	(2) <input type="checkbox"/>
pH 4.50	pH 4.50	pH 4.50	pH 4.50	pH 4.50	pH 4.50
Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2	Cryo1 2

3116

3118 **Move Up**

3120 **Move Down**

3122 **Delete**

3130 **Back** **Next >** **3132** **Cancel** **3134** **Help** **3136**

3116 **Well 7-**

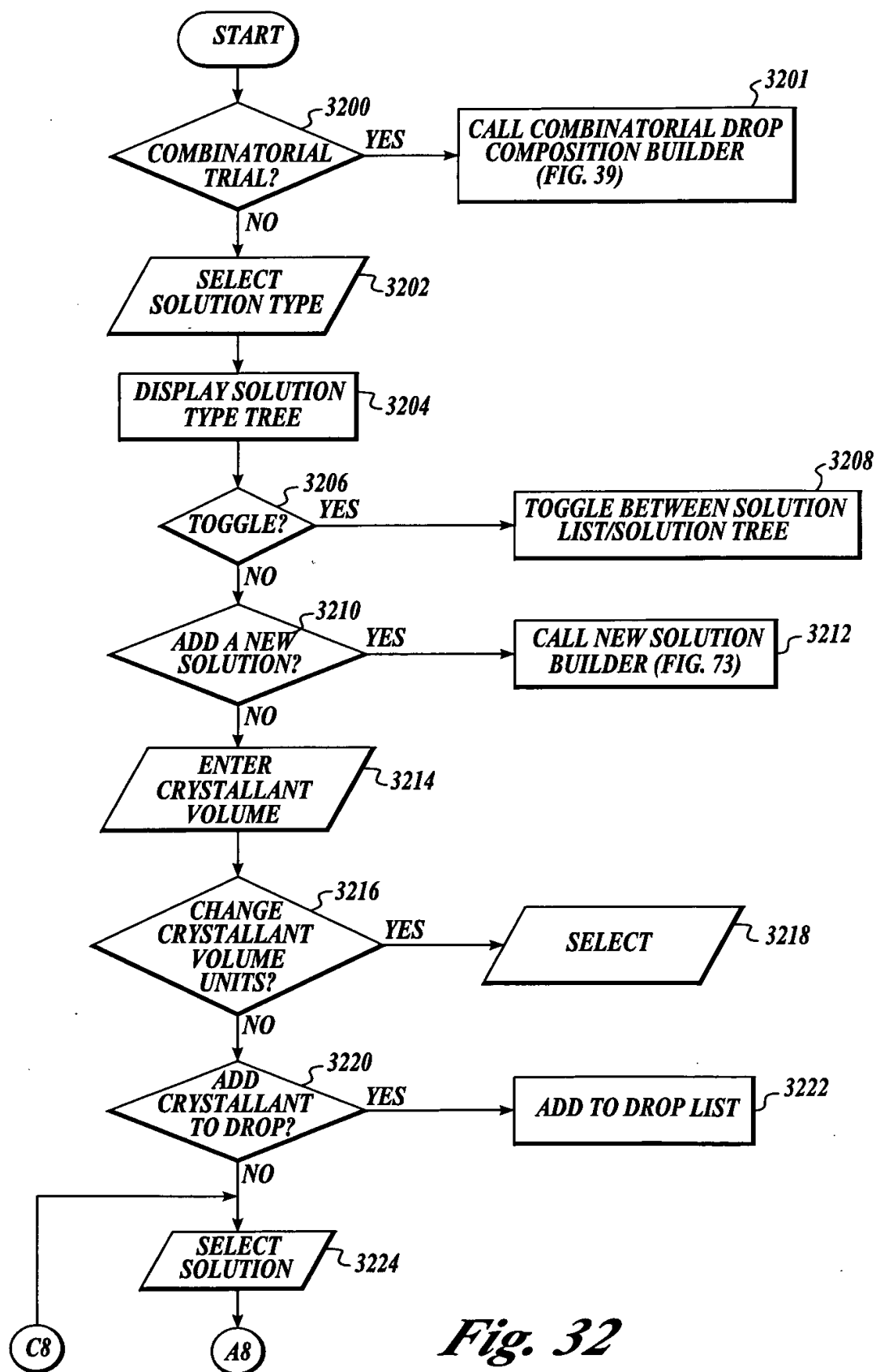
Compound Buffers:
100.000mM (acetic acid, NaAc) pH 4.50

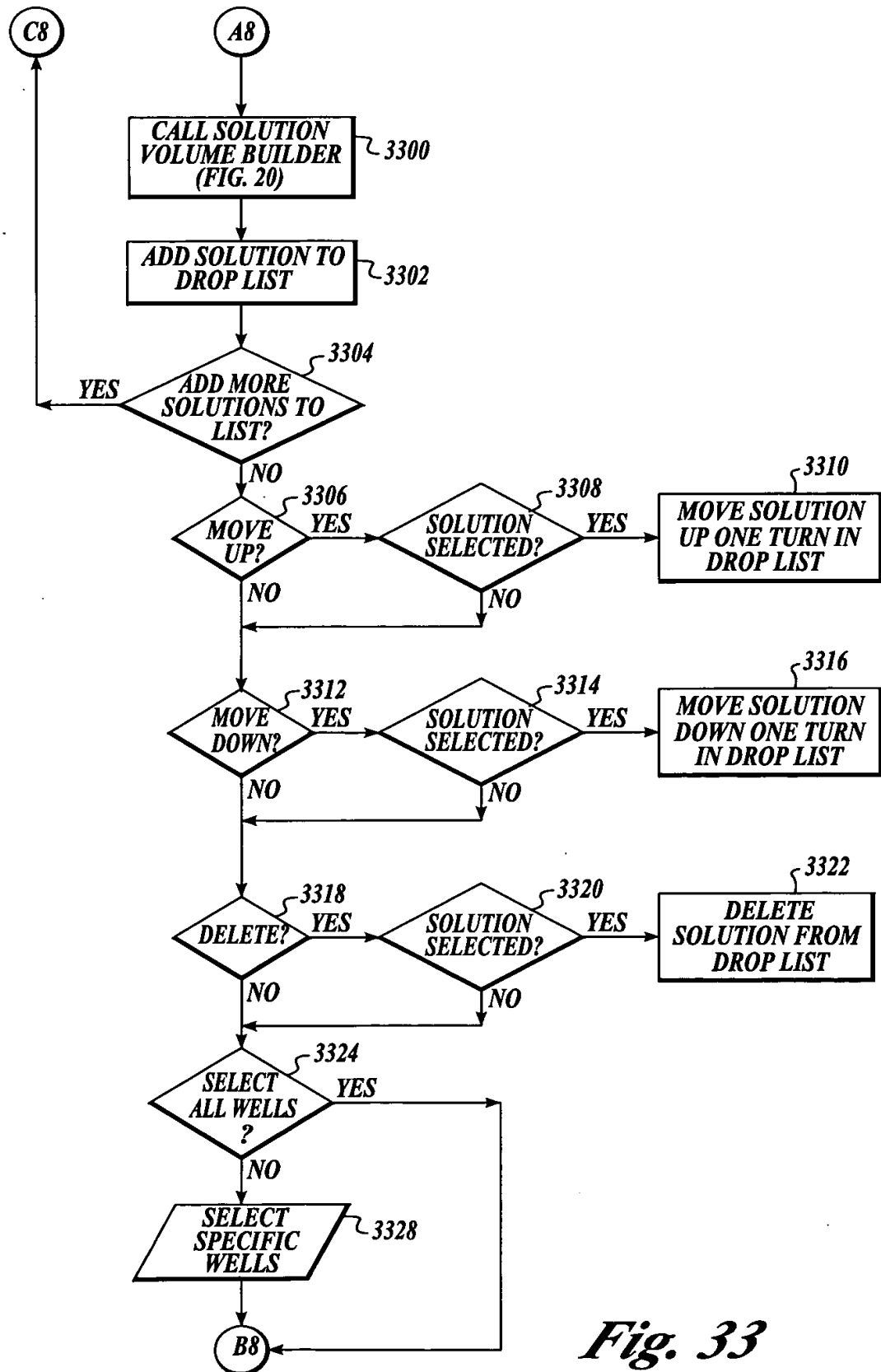
Chemicals:
40.000%v/v EG, Precipitant (Aldrich Chemical Co. 29,323-7)

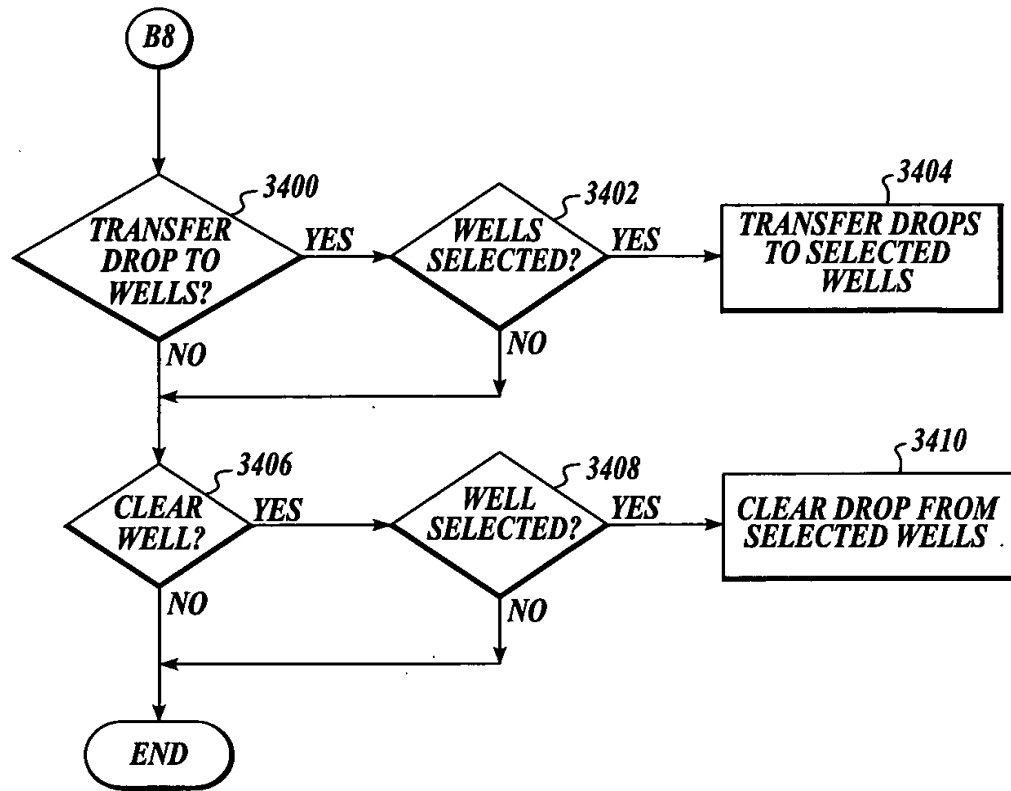
Crystallization Drop:
2.000 µl ijprotein040300
2.000 µl Crystallant

Solution Properties:
Final pH: 4.50 est.
Conductivity: n/a
Vapor Pressure Osmolality: n/a
Viscosity: Low
Solvent: H2O

Fig. 31

*Fig. 32*

*Fig. 33*

*Fig. 34*

3500

New Trial - Tray Barcode Assignment

Help

Enter each tray barcode either through keyboard or by using a barcode reader attached to COM port.

The hand points the tray that will receive barcode input next.

3501

10009999

Comment:

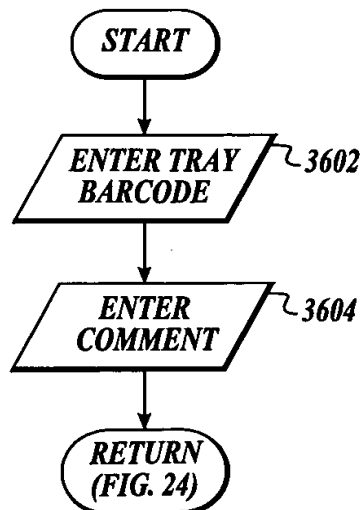
3502

jjprotein040300 in Cryo I #2, and jjprotein040300b in Cryo II #11

3510

< Back Finish Cancel Help

3504 3506 3508

Fig. 35*Fig. 36*

New Trial Wizard - Copy Well

Select Source Matrix

Wzrd1 (48 conditions)

pH 9.50	pH 7.50	pH 9.50	pH 8.00	pH 10.50	pH 5.50
pH 6.00	pH 5.50	pH 4.50	pH 7.00	pH 6.00	pH 8.00
pH 6.50	pH 6.50	pH 8.00	pH 6.20	pH 4.50	pH 8.00
pH 7.00	pH 8.00	pH 7.50	pH 8.50	pH 8.00	pH 7.00
pH 8.50	pH 9.50	pH 10.50	pH 7.50	pH 9.50	pH 4.50
pH 4.20	pH 6.20	pH 10.50	pH 8.00	pH 4.50	pH 8.00

Dilution(%): 100

Dilute sel

Clear

Sel all...

1

Copy

4x Combi Copy

VDX plate 4x combi

☒ 4x Combinatorial

pH 9.50 Wzrd1 1	pH 9.50 Wzrd1 1	pH 7.50 Wzrd1 2	pH 7.50 Wzrd1 2	pH 9.50 Wzrd1 3	pH 9.50 Wzrd1 3
pH 9.50 Wzrd1 1	pH 9.50 Wzrd1 1	pH 7.50 Wzrd1 2	pH 7.50 Wzrd1 2	pH 9.50 Wzrd1 3	pH 9.50 Wzrd1 3
pH 6.00 Wzrd1 7	pH 6.00 Wzrd1 7	pH 5.50 Wzrd1 8	pH 5.50 Wzrd1 8	pH 4.50 Wzrd1 9	pH 4.50 Wzrd1 9
pH 6.00 Wzrd1 7	pH 6.00 Wzrd1 7	pH 5.50 Wzrd1 8	pH 5.50 Wzrd1 8	pH 4.50 Wzrd1 9	pH 4.50 Wzrd1 9
pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 14	pH 6.50 Wzrd1 14	pH 8.00 Wzrd1 15	pH 8.00 Wzrd1 15

Back

Next >

Cancel

Help

Emerald's Wizard I Crystal Growth Matrix. A random sparse matrix of crystallants (1-48).

Fig. 37

3800 New Trial Wizard - Drop Composition

☐ Additive
☐ Formulation
☐ HeavyAtom
☐ Buffer Solution
☐ Stock Solution
☒ Macromol. Form.
☐ Cplx. Macromol.

asdert
 qwe
 wer
 yz4810

Crystallant
 Vol: 2

Volume Name
 2.00 µl yz4810
 2.00 µl Crystallant

3801

CombiClover

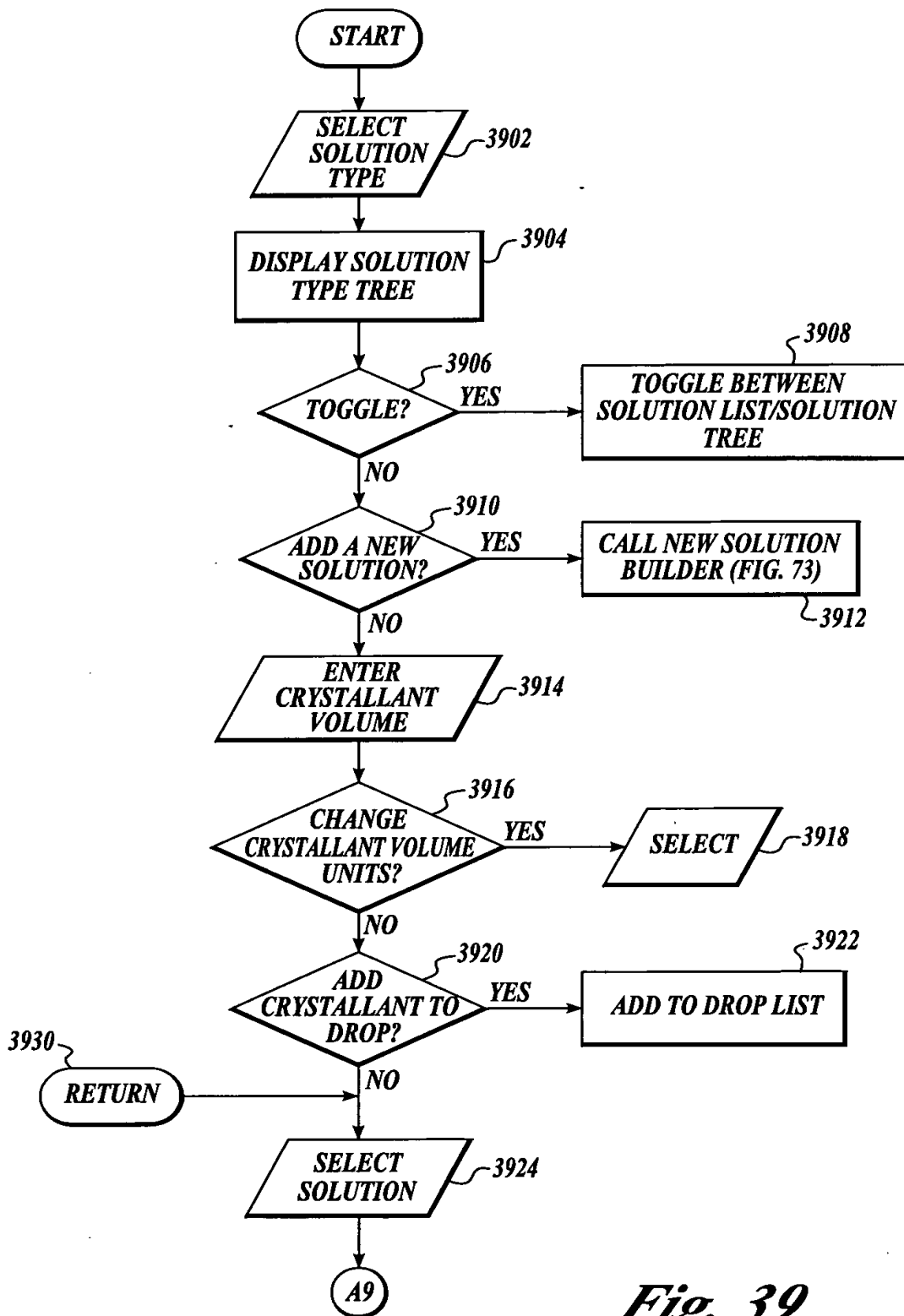
(2)▲ pH 9.50 Wzrd1 1	(2) pH 9.50 Wzrd1 1	(3)▲ pH 7.50 Wzrd1 2	(2)▲ pH 7.50 Wzrd1 2	(2) pH 9.50 Wzrd1 3
(2) pH 9.50 Wzrd1 1	(2) pH 9.50 Wzrd1 1	(3) pH 7.50 Wzrd1 2	(3) pH 7.50 Wzrd1 2	(2) pH 9.50 Wzrd1 3
(2)▲ pH 6.00 Wzrd1 7	(2) pH 6.00 Wzrd1 7	(2)▲ pH 5.50 Wzrd1 8	(2)▲ pH 5.50 Wzrd1 8	(2) pH 4.50 Wzrd1 9
(3) pH 6.00 Wzrd1 7	(3) pH 6.00 Wzrd1 7	(2) pH 5.50 Wzrd1 8	(2) pH 5.50 Wzrd1 8	(2) pH 4.50 Wzrd1 9
(2)▲ pH 6.50 Wzrd1 13	(2) pH 6.50 Wzrd1 13	(2)▲ pH 6.50 Wzrd1 14	(2)▲ pH 6.50 Wzrd1 14	(2) pH 8.00 Wzrd1 15
pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 13	pH 6.50 Wzrd1 14	pH 6.50 Wzrd1 14	pH 8.00 Wzrd1 15

3804 3806 3808 3810

Transfer Drop to sel. Wells

3802

Fig. 38

*Fig. 39*

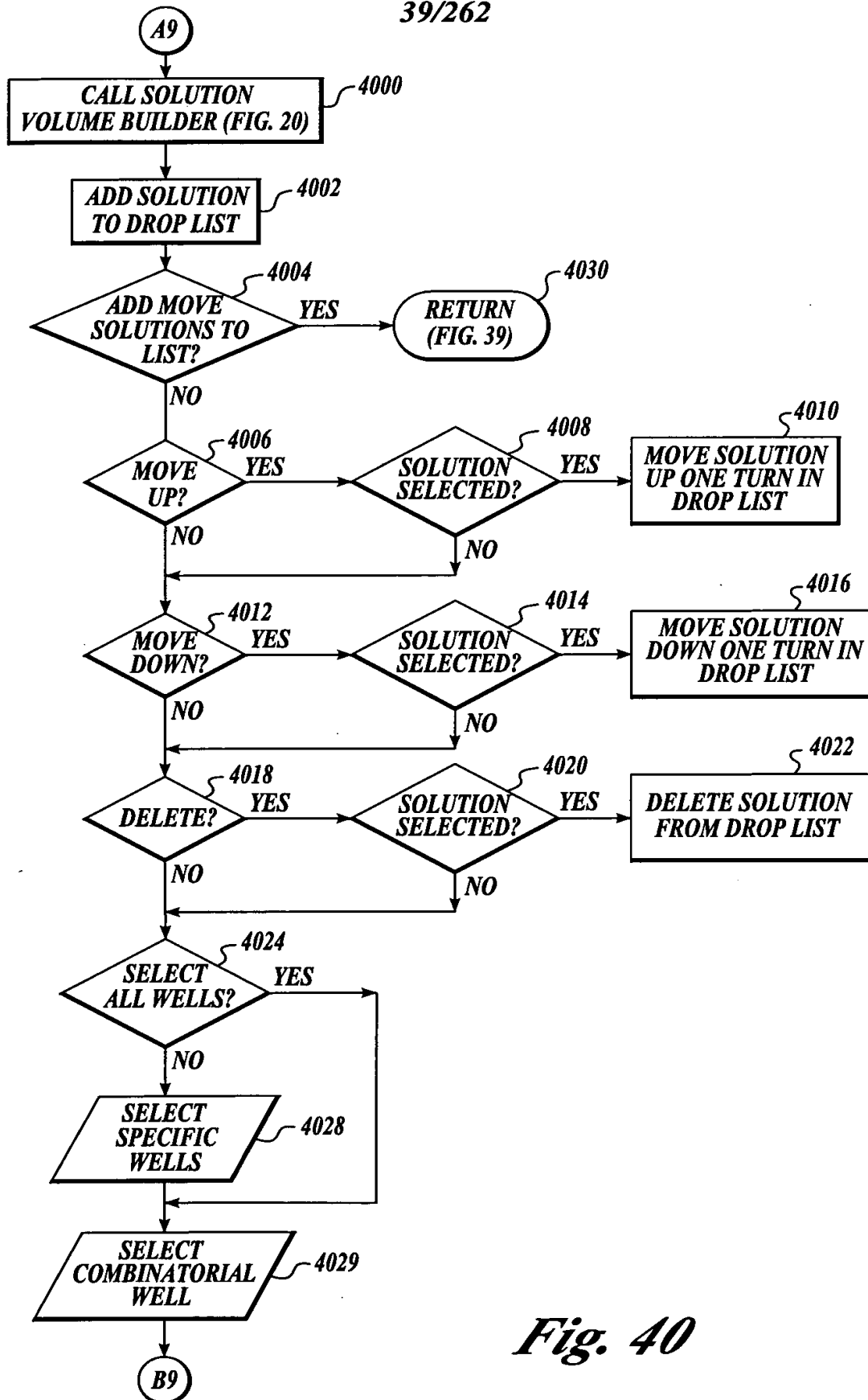
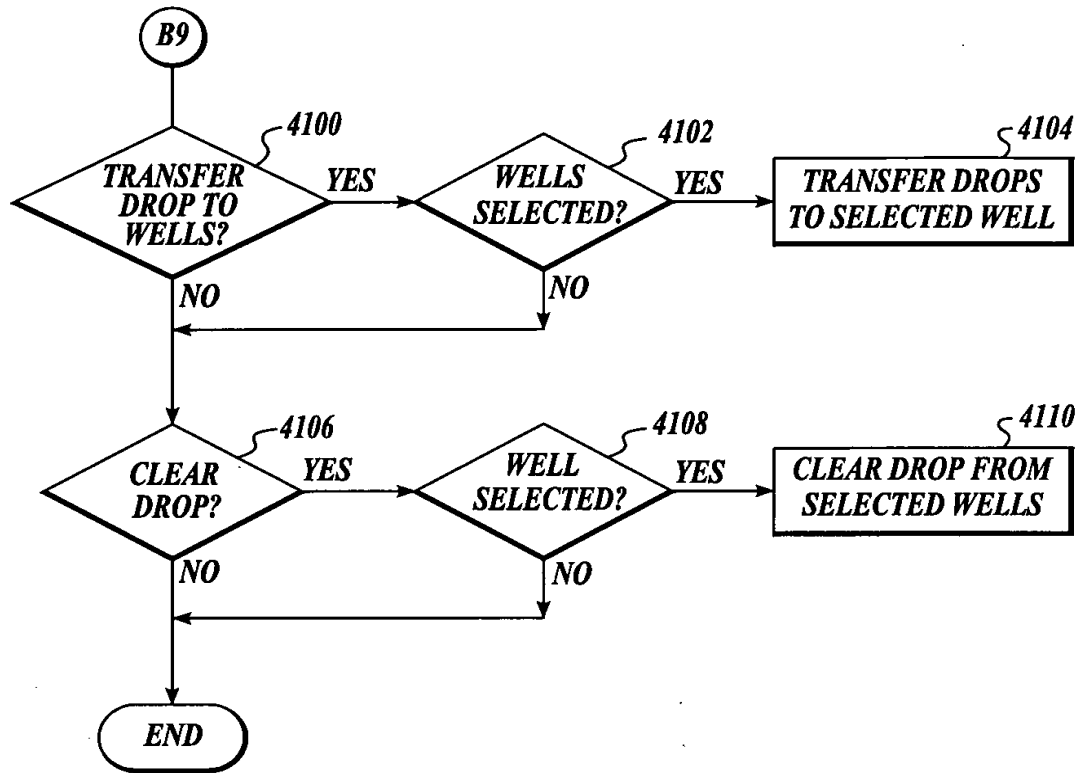
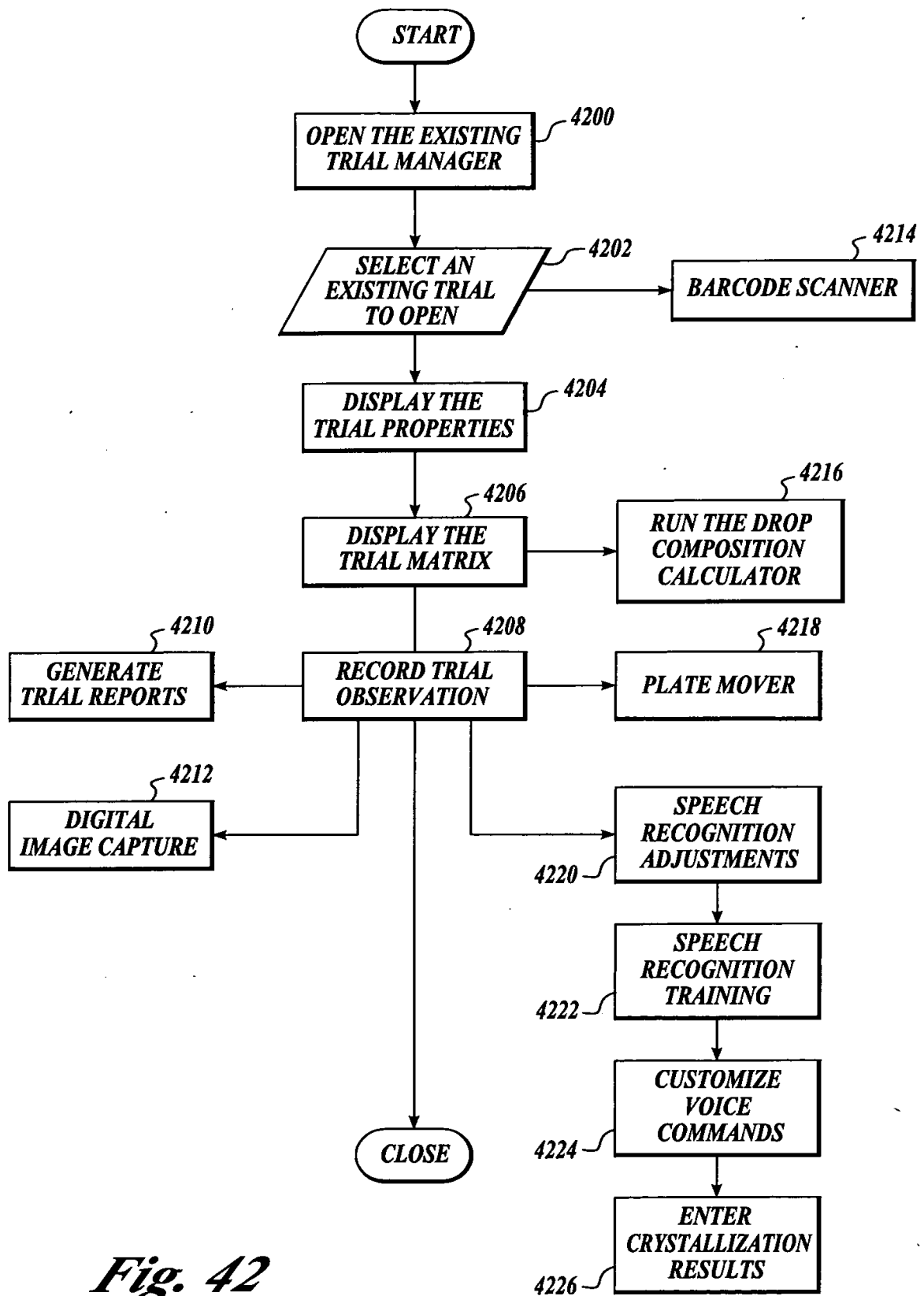


Fig. 40

*Fig. 41*

*Fig. 42*

4300 { 4304 { 4302 { 4306 { 4308 {

Open Trial

From: Tuesday, January 04, 2000 [v] Until: Tuesday, April 04, 2000 [v] Query!

TrialID	TrialType	ObservationSessions	UserName	SetupDate	ProjectName	Tempe
5	Complex	0	Admin	4/3/2000 17:....	ijiprotein	25 C
4	Complex	0	Admin	4/3/2000 16:....	ijiprotein	25 C
3	Normal	0	Admin	4/3/2000 16:....	test	25 C
2	Normal	1	Admin	4/3/2000 11:....	test	25 C
1	Normal	2	Admin	3/22/2000 1:....	test	25 C

4301

Select one or more trials and click OK or use barcode reader to load a trial. The barcode reader is activated as long as the dialog is active.

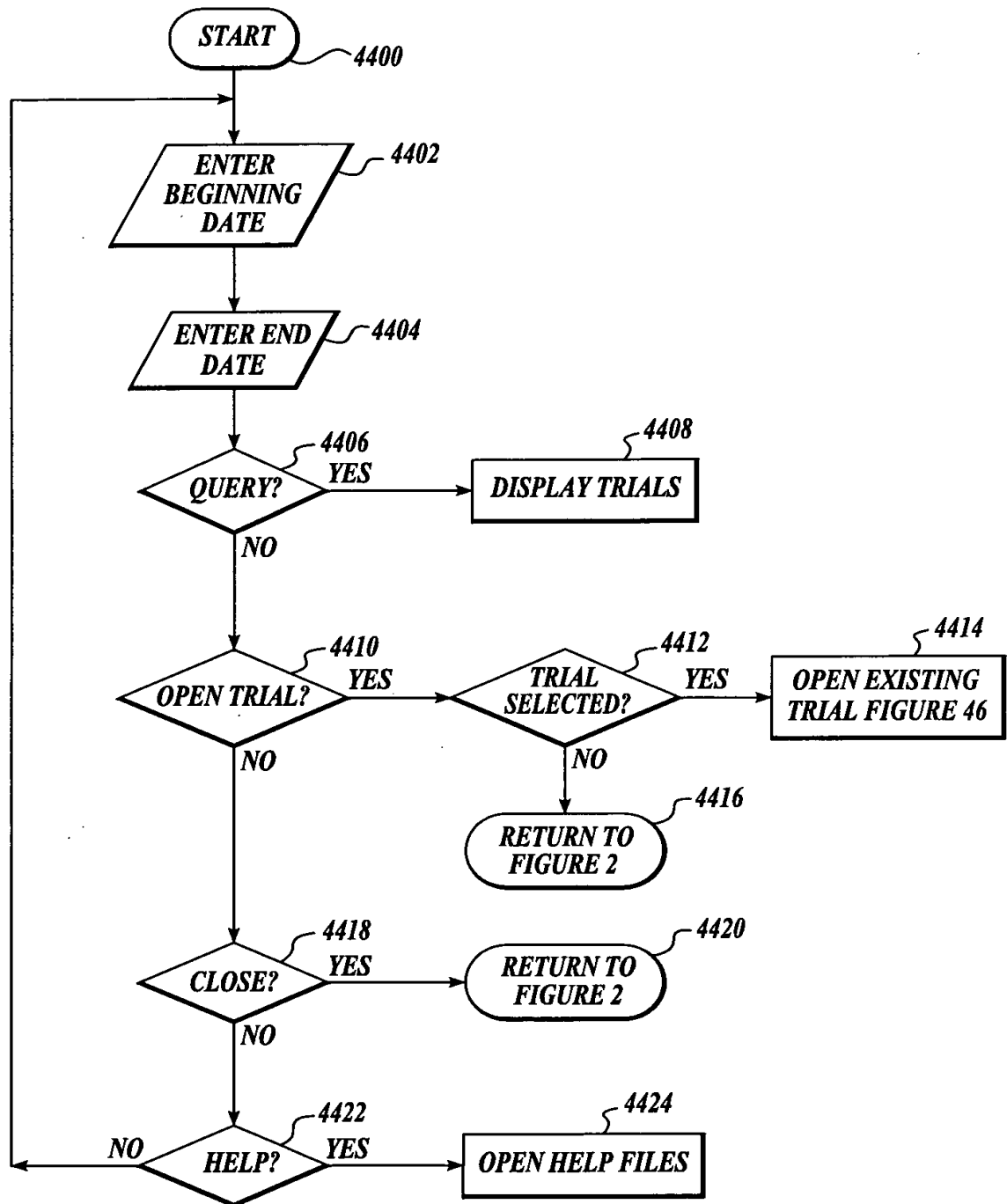
5 Trial(s) have been created between the specified dates.

4312 { 4314 { 4316 {

Open

Help

Fig. 43

*Fig. 44*

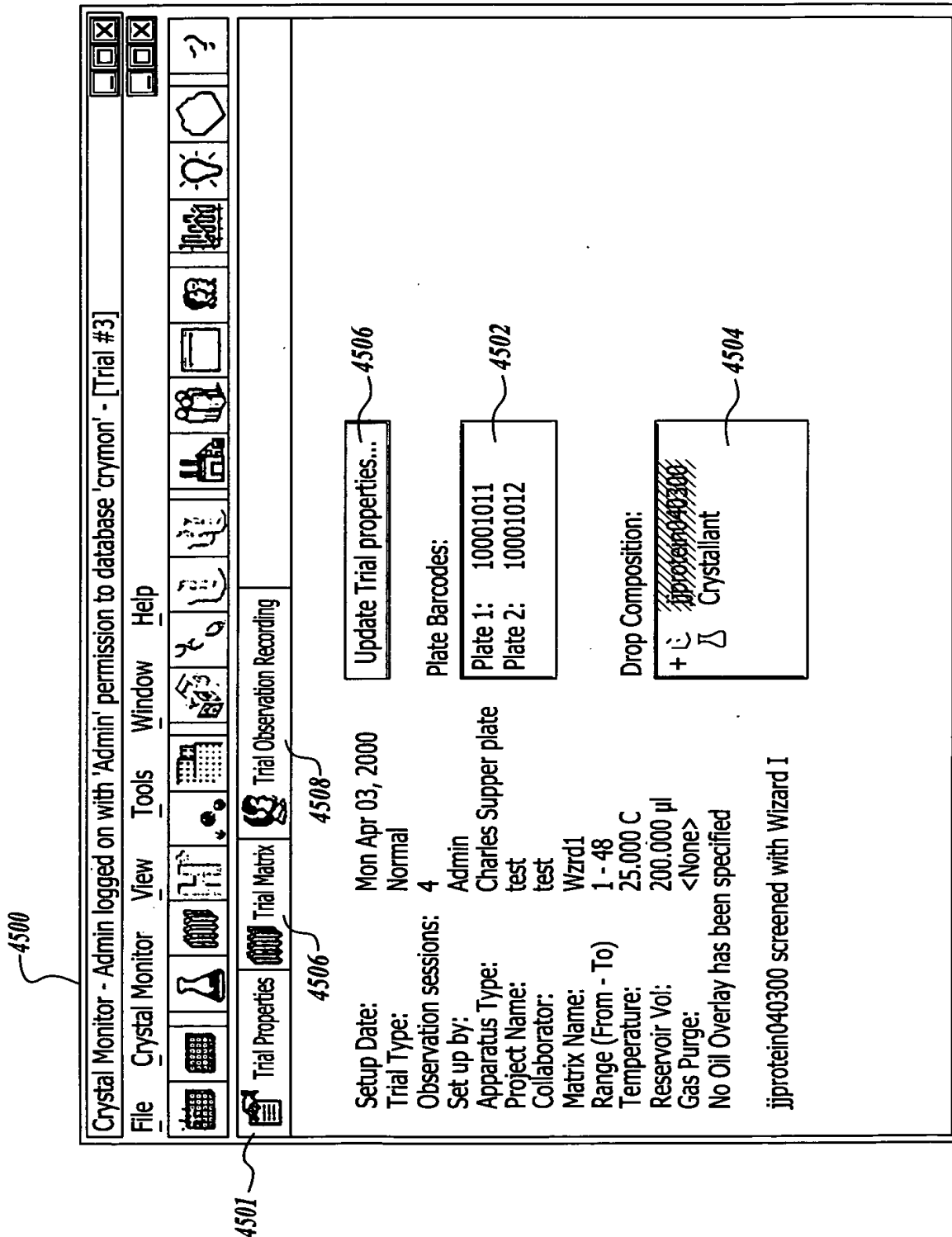
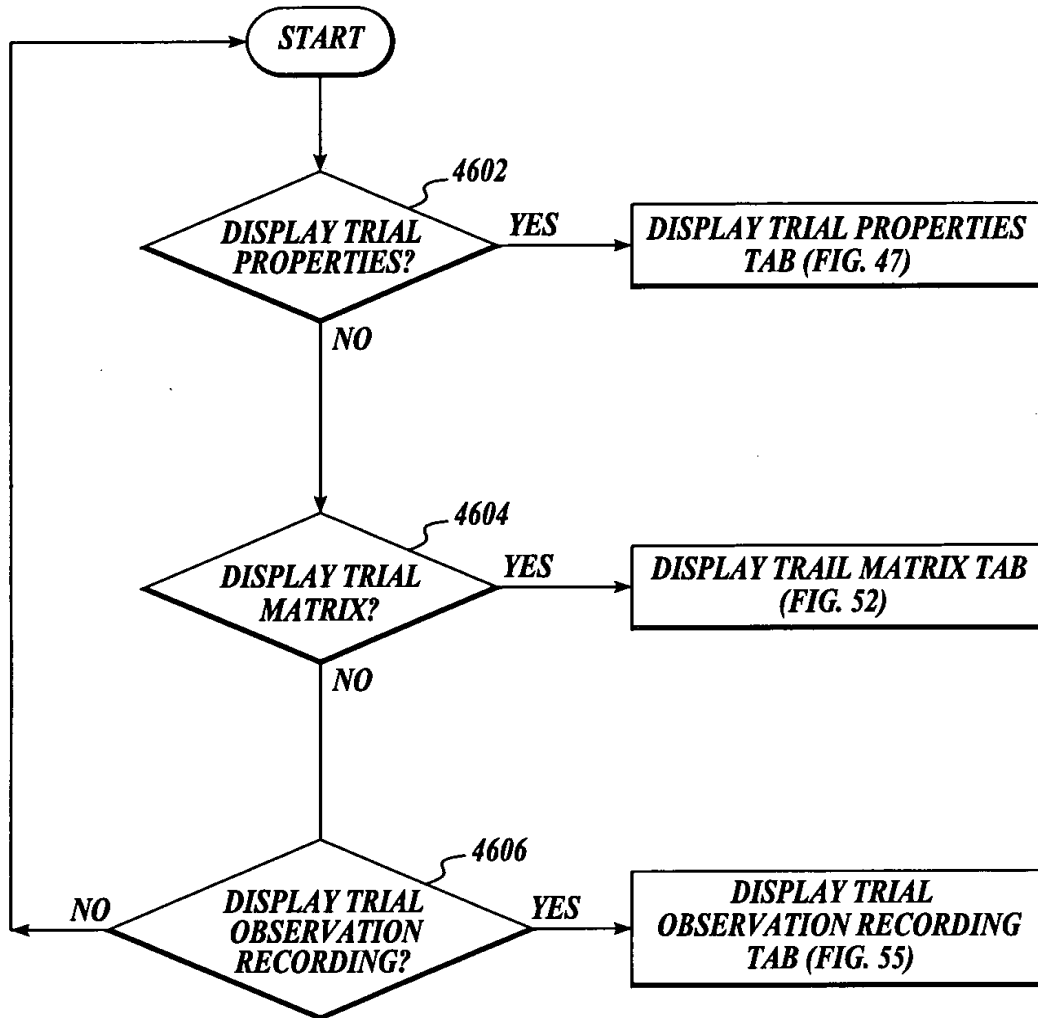
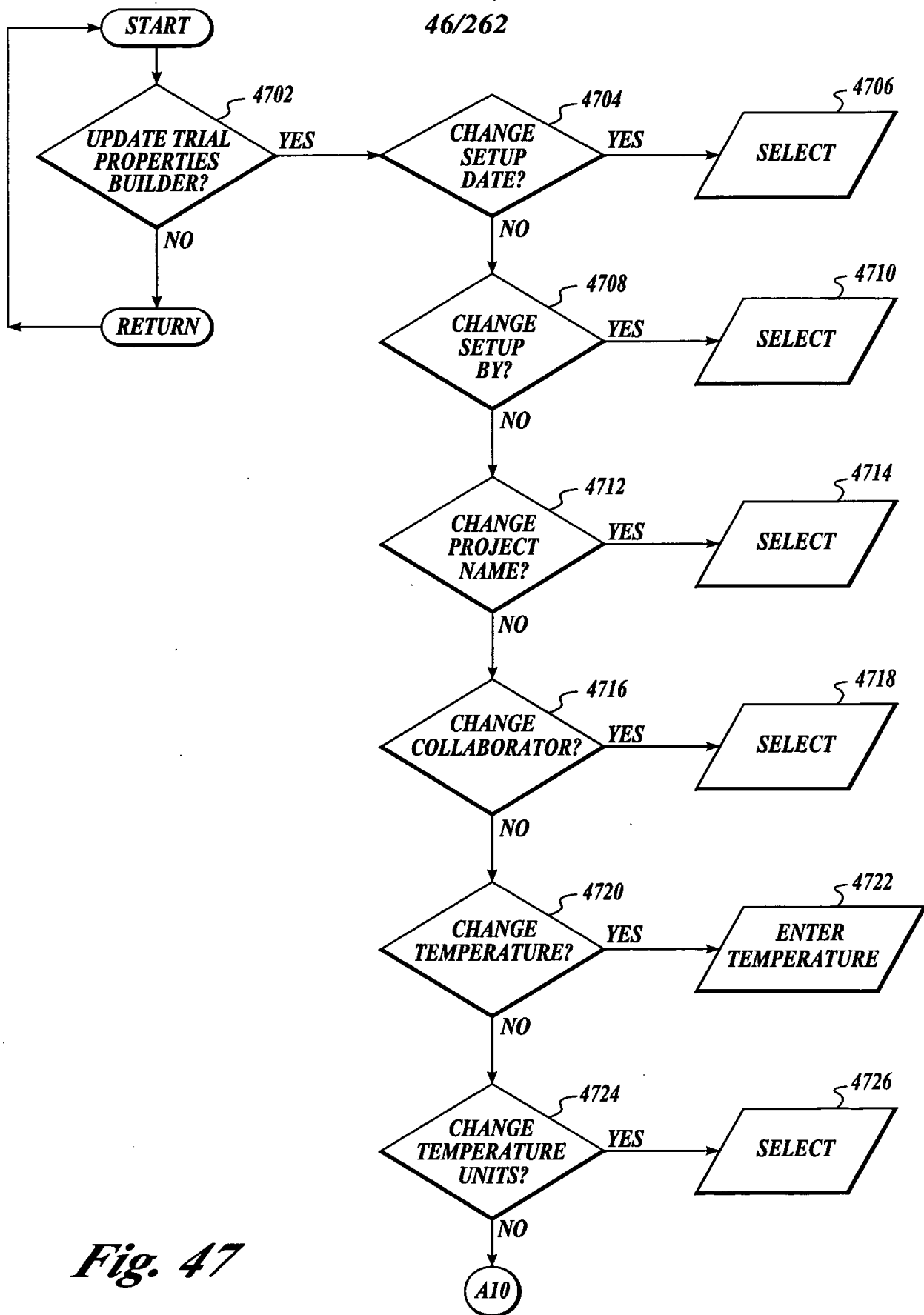
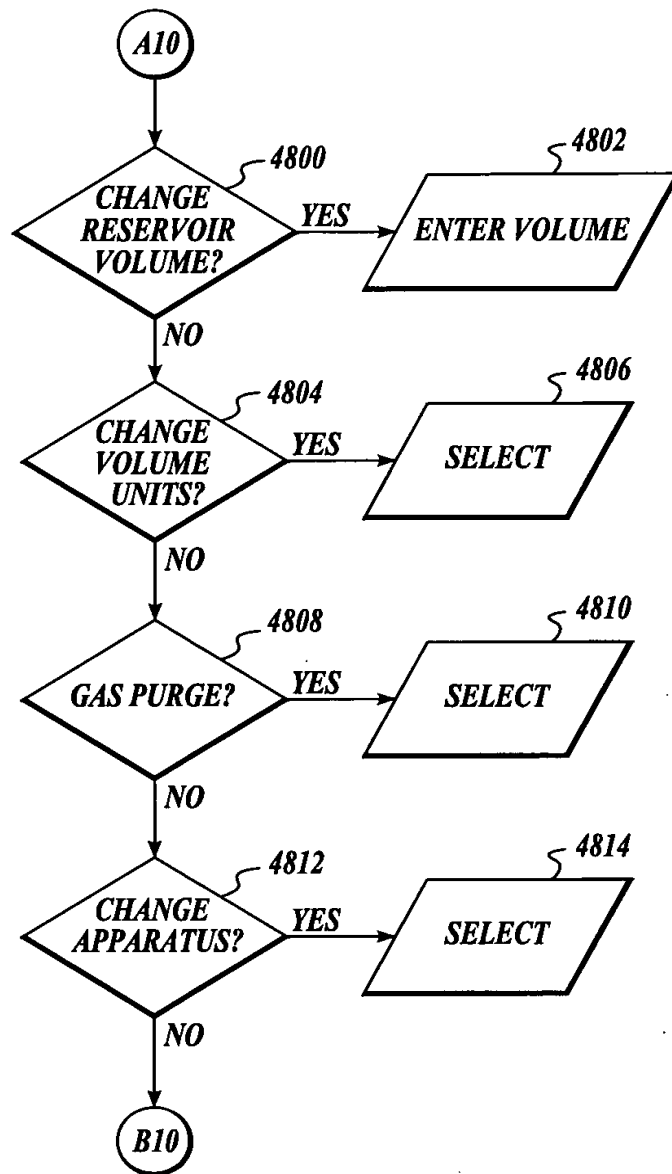
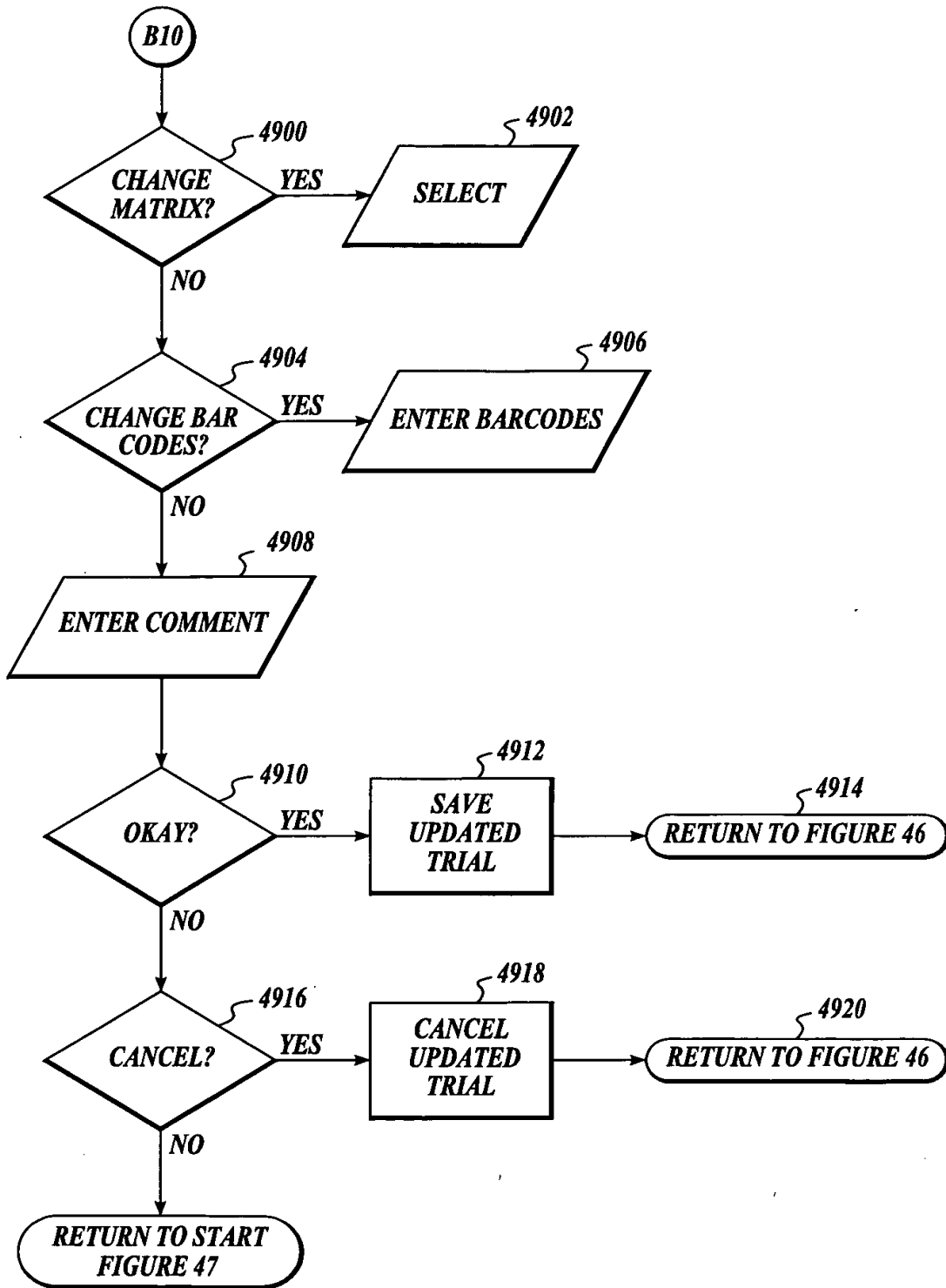


Fig. 45

*Fig. 46*



*Fig. 48*

*Fig. 49*

5000 Crystal Monitor - Admin logged on with 'Admin' permission to database 'crymon' - [Trial #3]

File Crystal Monitor View Tools Window Help

5002

5004

Trial Properties

pH 9.50	pH 7.50	pH 9.50	pH 8.00	pH 10.50	pH 5.50
pH 6.00	pH 5.50	pH 4.50	pH 7.00	pH 6.00	pH 8.00

Trial Matrix

Trial Observation Recording

Matrix Name: Wzrd1

Matrix Type: Random

Commercial:

Compound Buffers:
100.000mM (Na3 citrate, citric acid) pH 5.50

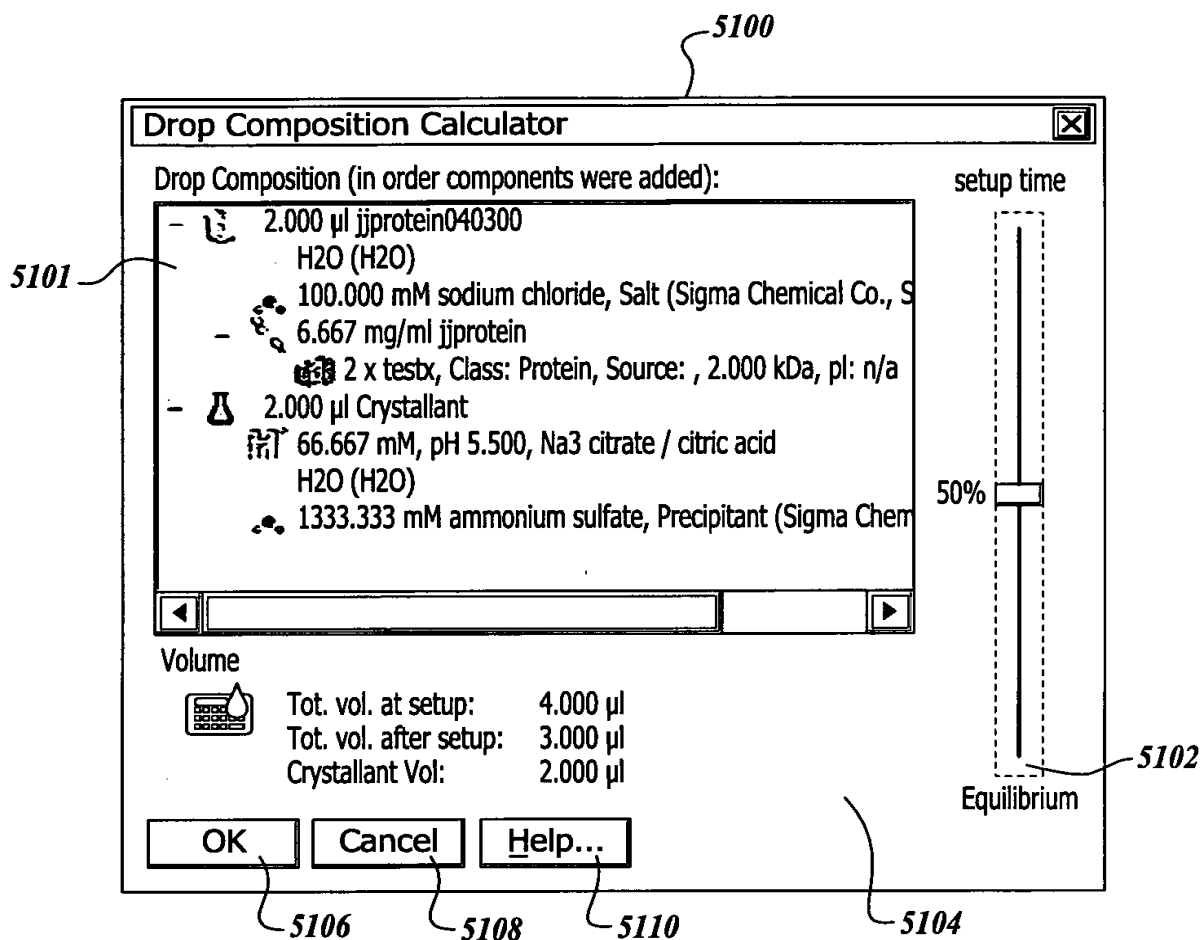
Chemicals:
2000.000 Mm (NH4)2 sulfate, Precipitant (Sigma Chemical Co. A2939)

Crystallization Drop:
2.000 μ l jprotein040300
2.000 μ l Crystallant

Solution Properties:
Final pH: 5.50 est.
Conductivity: n/a
Vapor Pressure Osmolality: n/a
Viscosity: Low
Solvent: H2O

uctures, Inc.
atically varied);
atically varied);
ard Crystal Growth Matrix
se matrix of crystallants

Fig. 50

*Fig. 51*

51/262

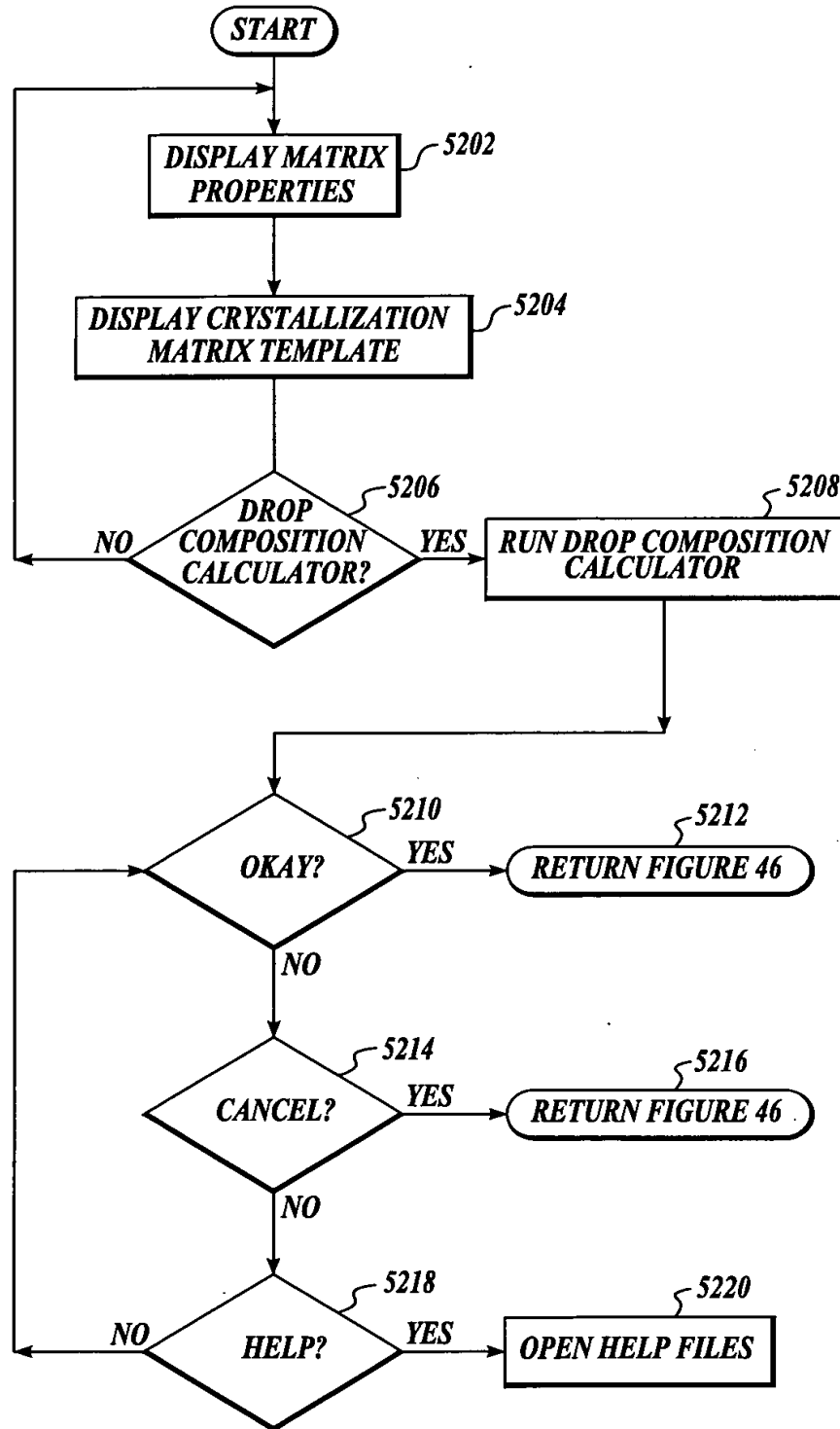


Fig. 52

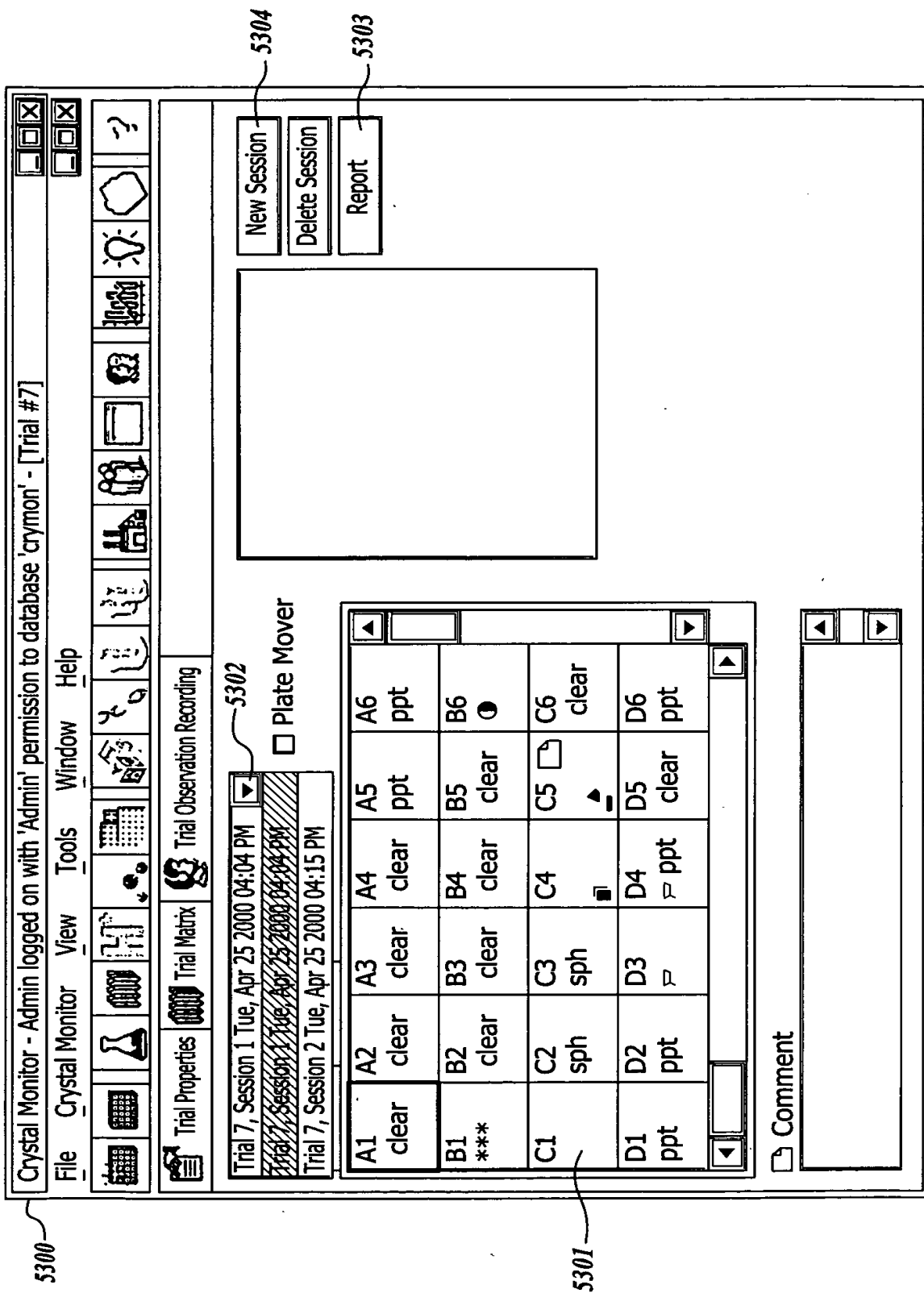


Fig. 53

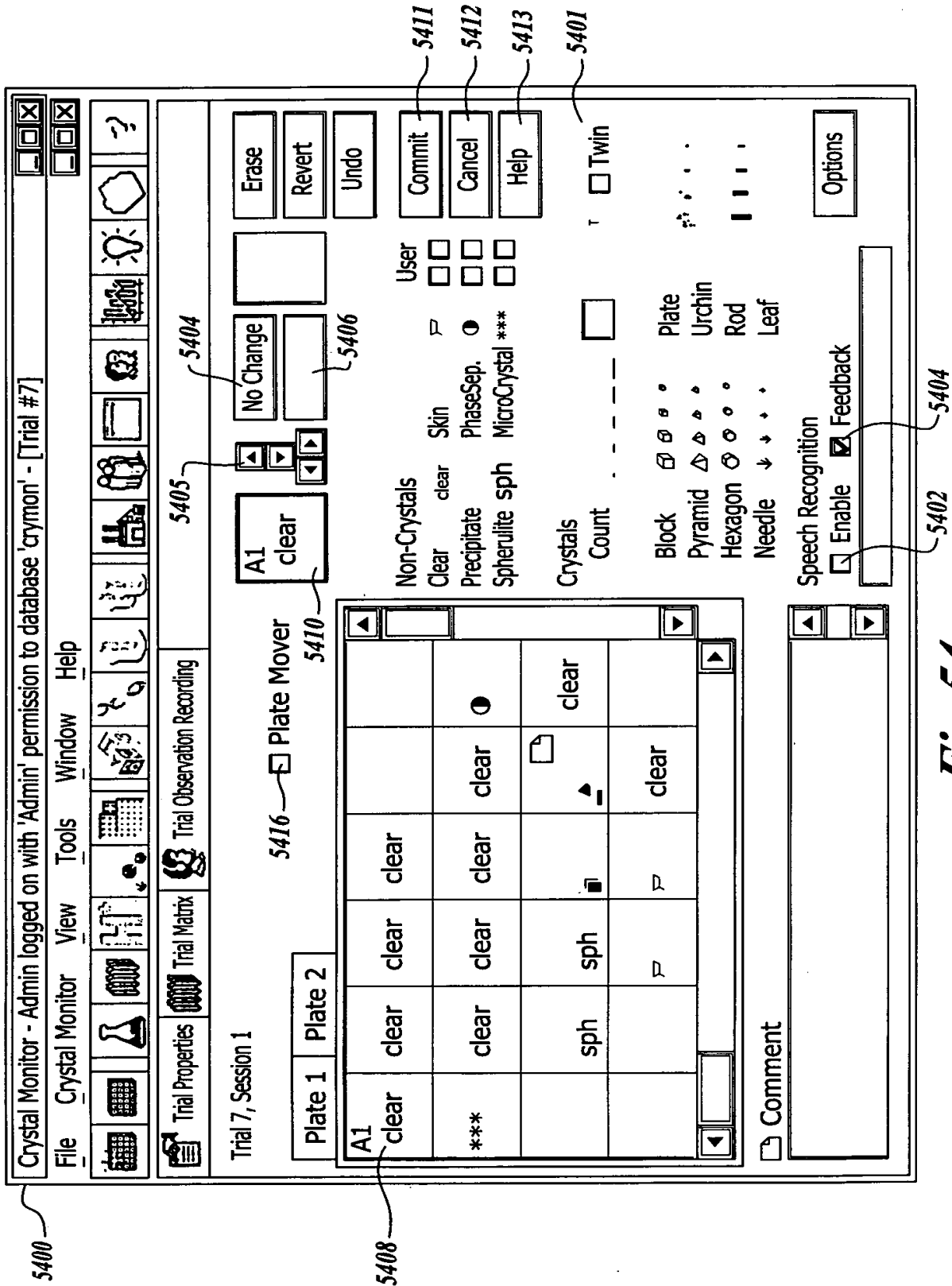


Fig. 54

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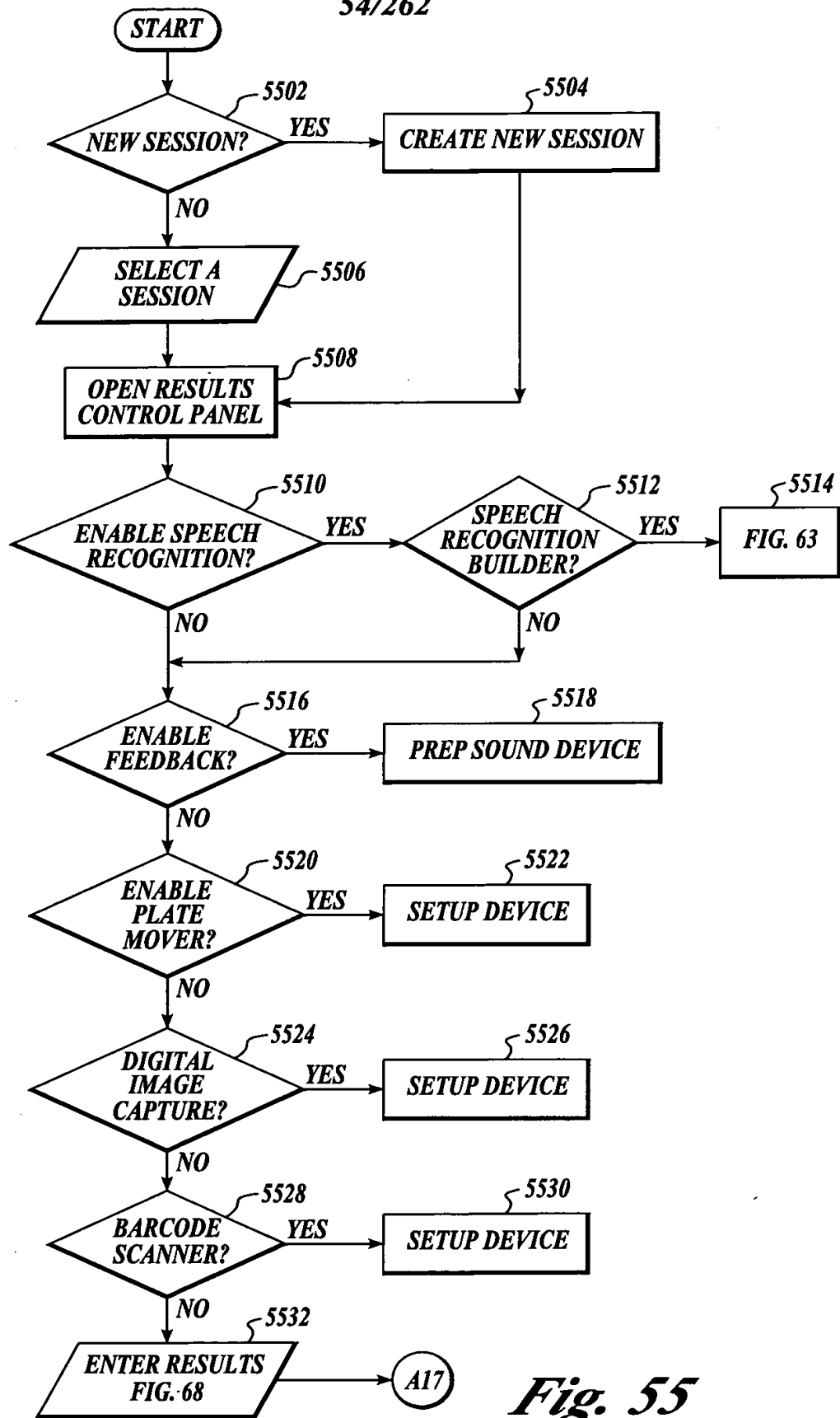
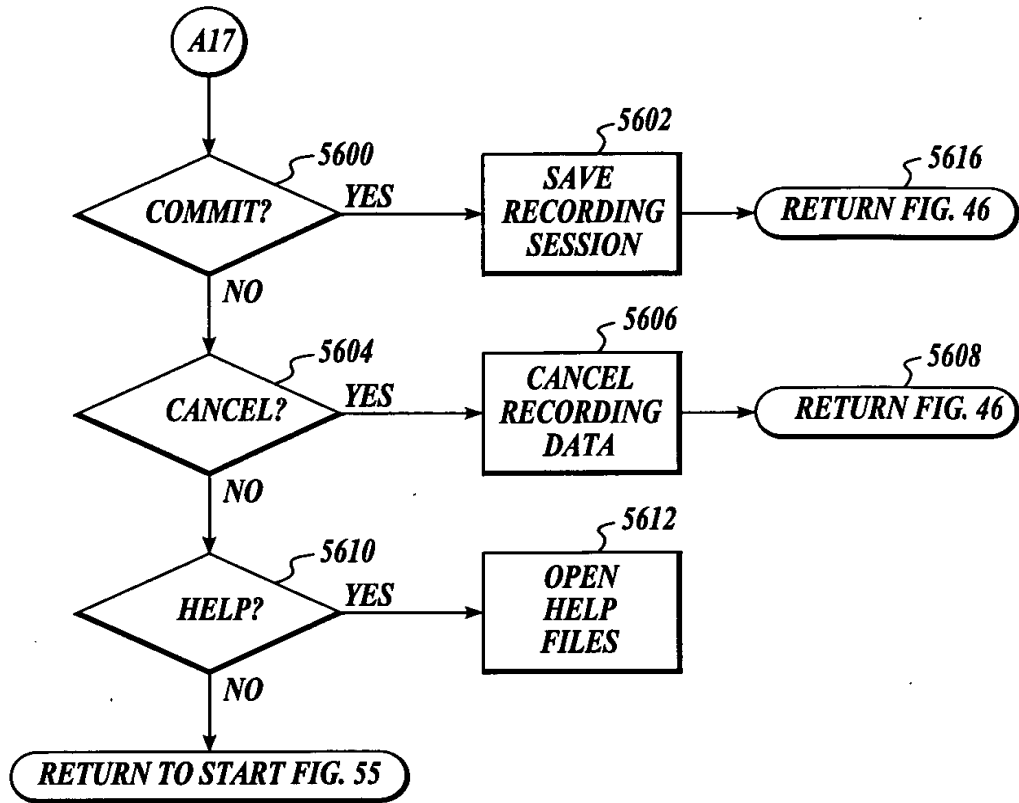
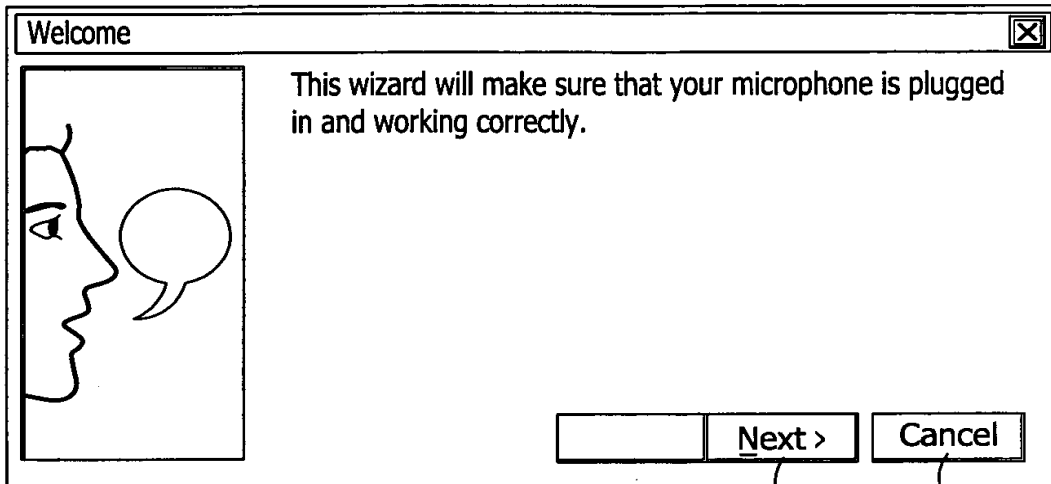


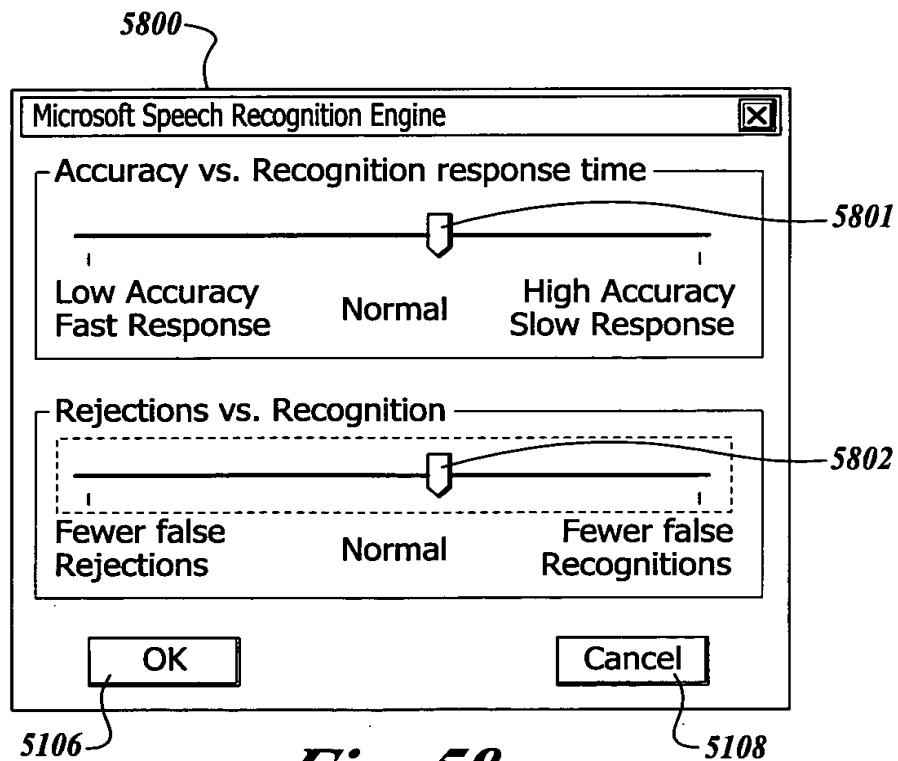
Fig. 55

*Fig. 56*



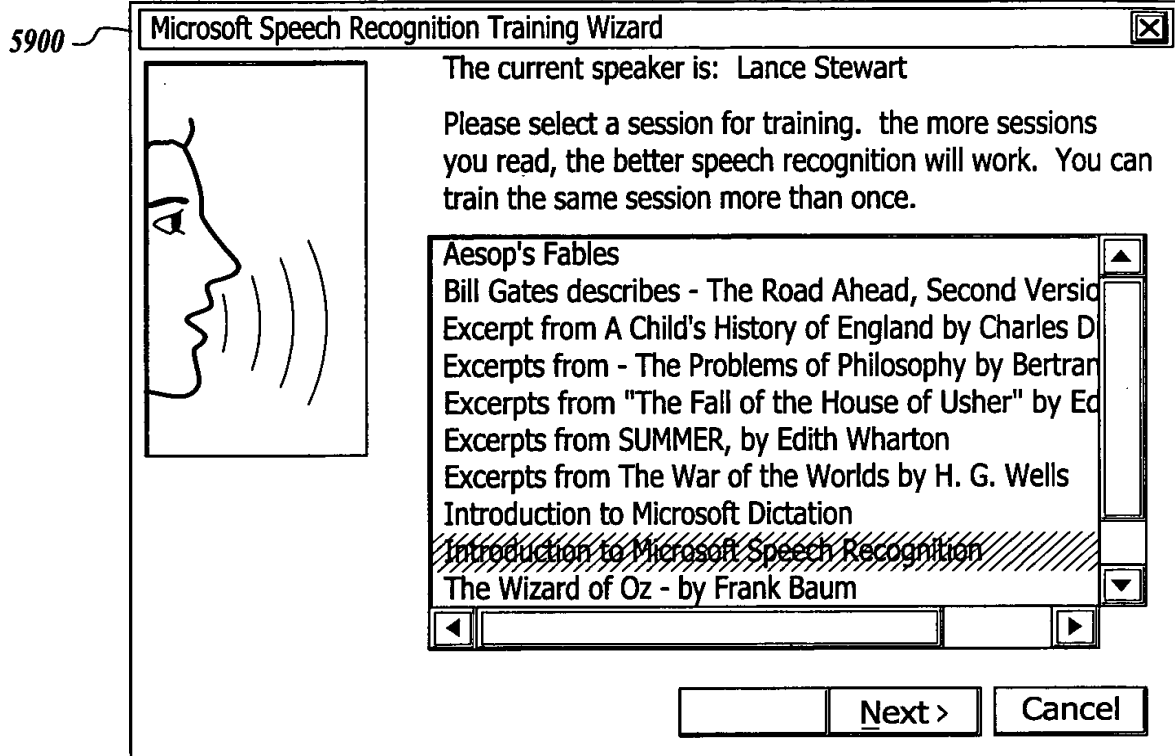
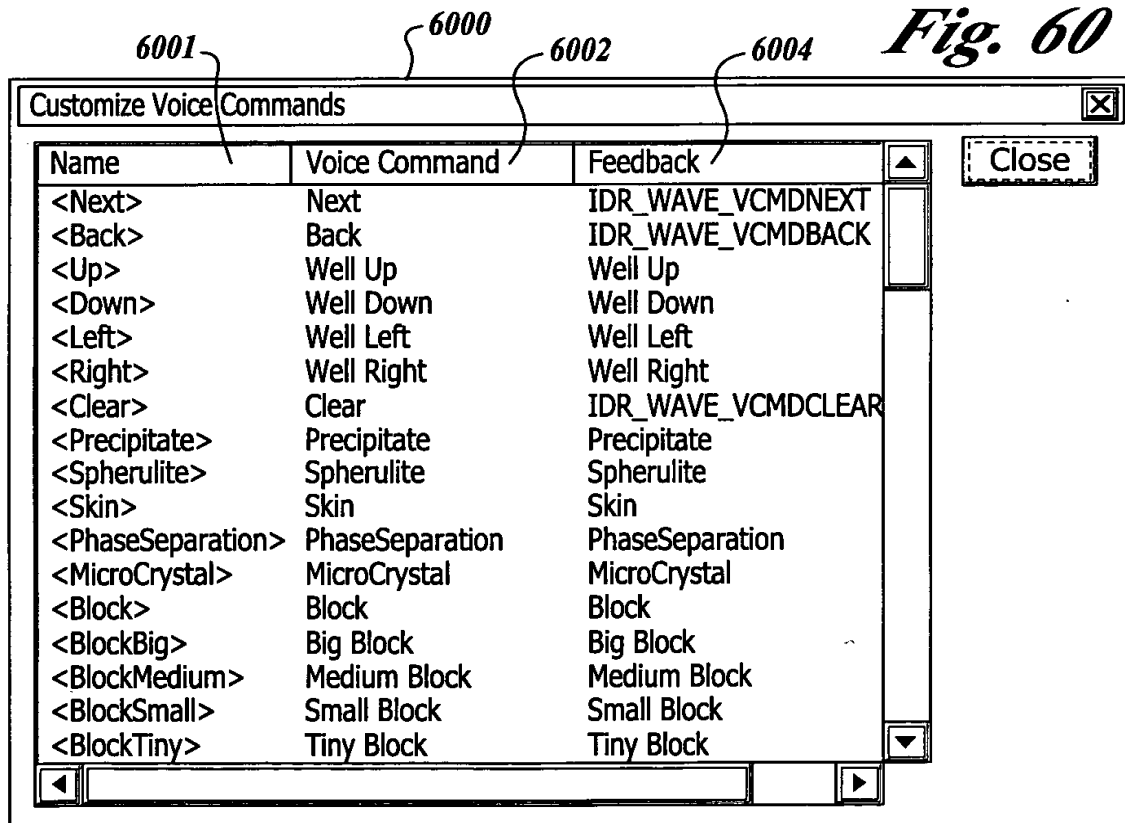
5700 *Fig. 57*

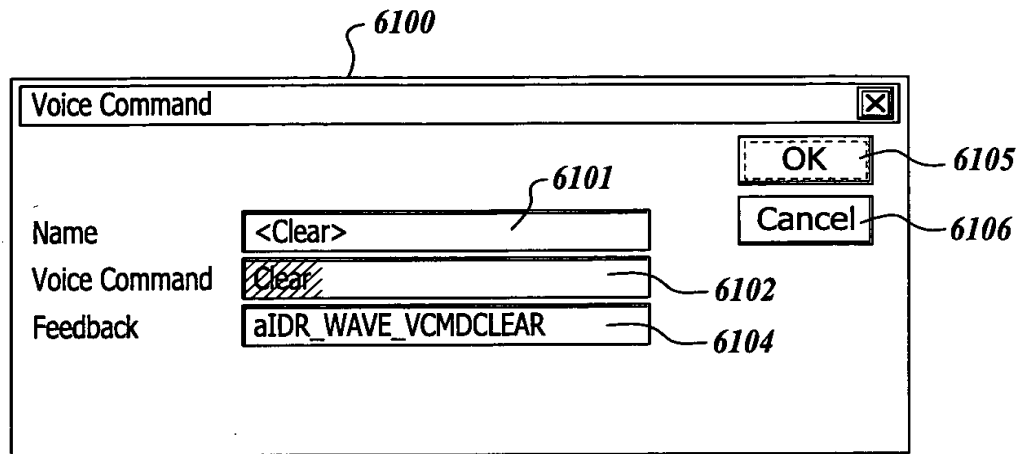
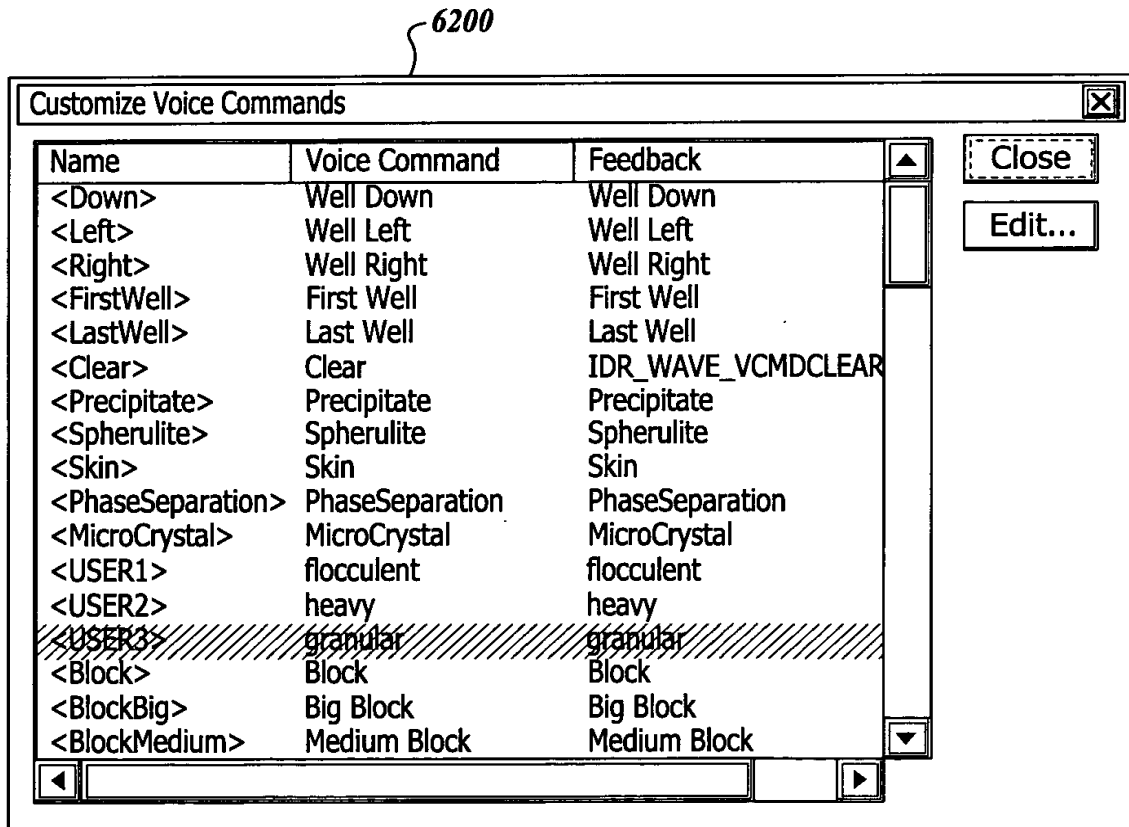
5702 5704

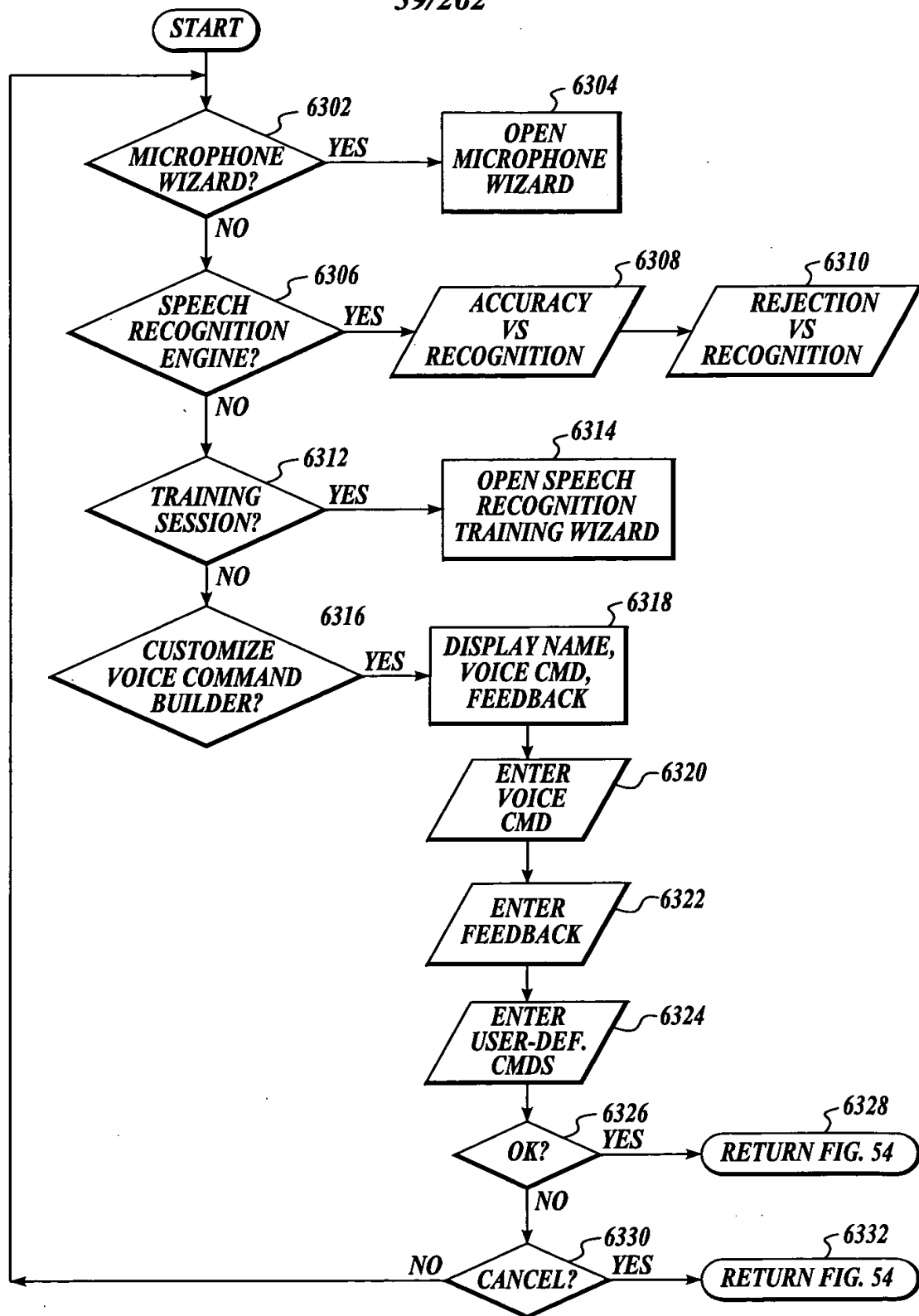


5106 *Fig. 58*

5108

*Fig. 59**Fig. 60*

*Fig. 61**Fig. 62*

*Fig. 63*

6400

Options

Barcode Reader Plate Mover Miscellaneous

COM PORT COM1

BAUD 9600 (def)

Stop Bits
☒ 1 (default)
☐ 2

Parity
☒ None (default)
☐ Even
☐ Odd

Testing
☒ Plate Mover ON for Testing

Command: p 0 0 0 Run

Response:

Align Co-ordinates Set Defaults

OK Cancel

6401

6402

Fig. 64



Fig. 65

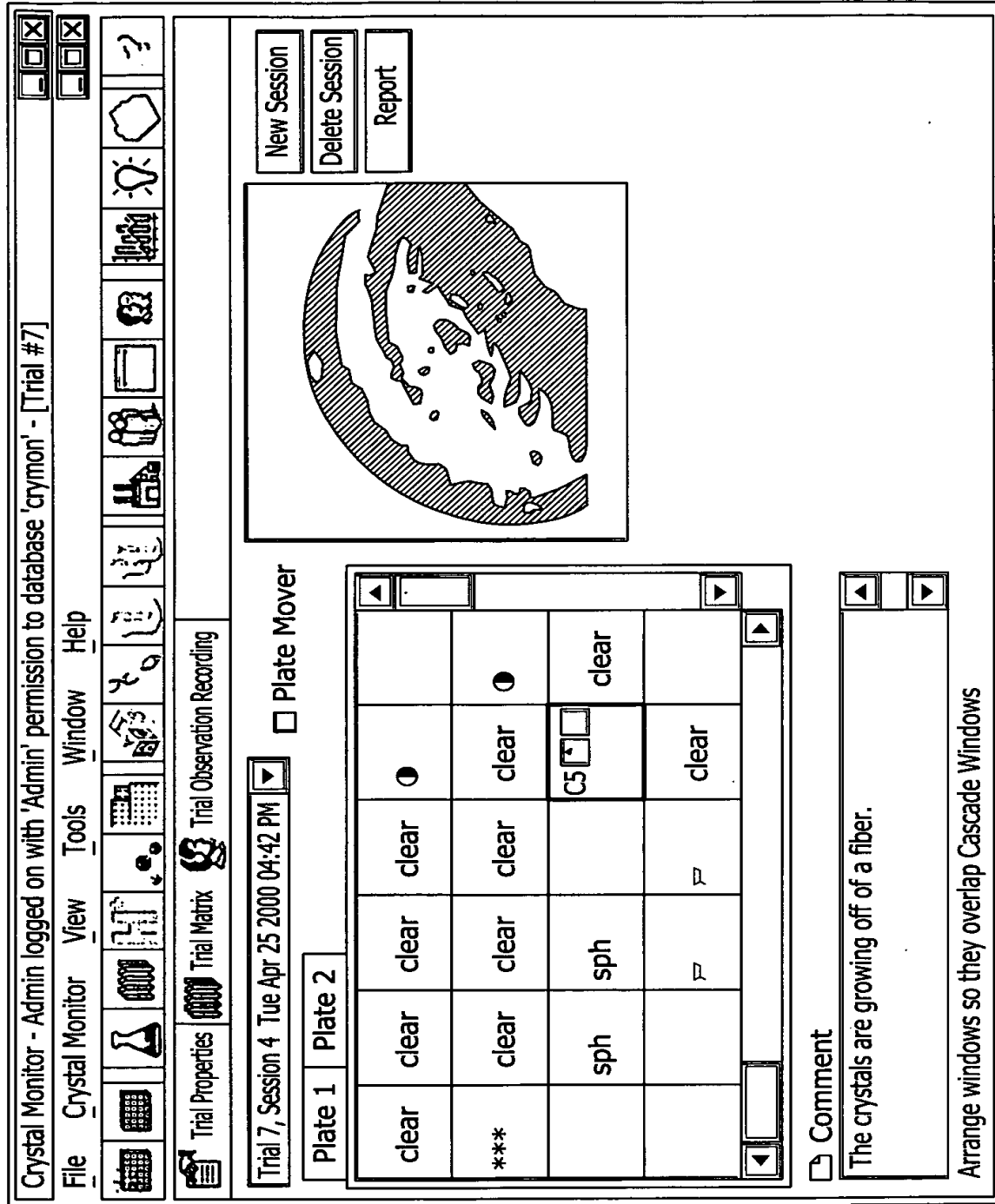


Fig. 66

6700

The image shows a software dialog box titled "Options" with a standard Windows-style title bar containing a question mark and a close button. The dialog has three tabs: "Barcode Reader", "Plate Mover", and "Miscellaneous". The "Barcode Reader" tab is currently selected. Inside this tab, there are two dropdown menus: "COM PORT" set to "COM1" and "BAUD" set to "9600 (def)". Below these are two groups of radio buttons. The "Stop Bits" group has "1 (default)" selected, with "2" as an alternative. The "Parity" group has "None (default)" selected, with "Even" and "Odd" as alternatives. There is a checked checkbox labeled "Barcode Reader ON for Testing". Below this is a text field labeled "Scanned Barcode:". In the bottom right corner of the dialog area is a button labeled "Set Defaults". At the very bottom of the dialog are three buttons: "OK", "Cancel", and an empty button.

Options

Barcode Reader Plate Mover Miscellaneous

COM PORT: COM1

BAUD: 9600 (def)

Stop Bits:

- ☒ 1 (default)
- ☐ 2

Parity:

- ☒ None (default)
- ☐ Even
- ☐ Odd

Testing:

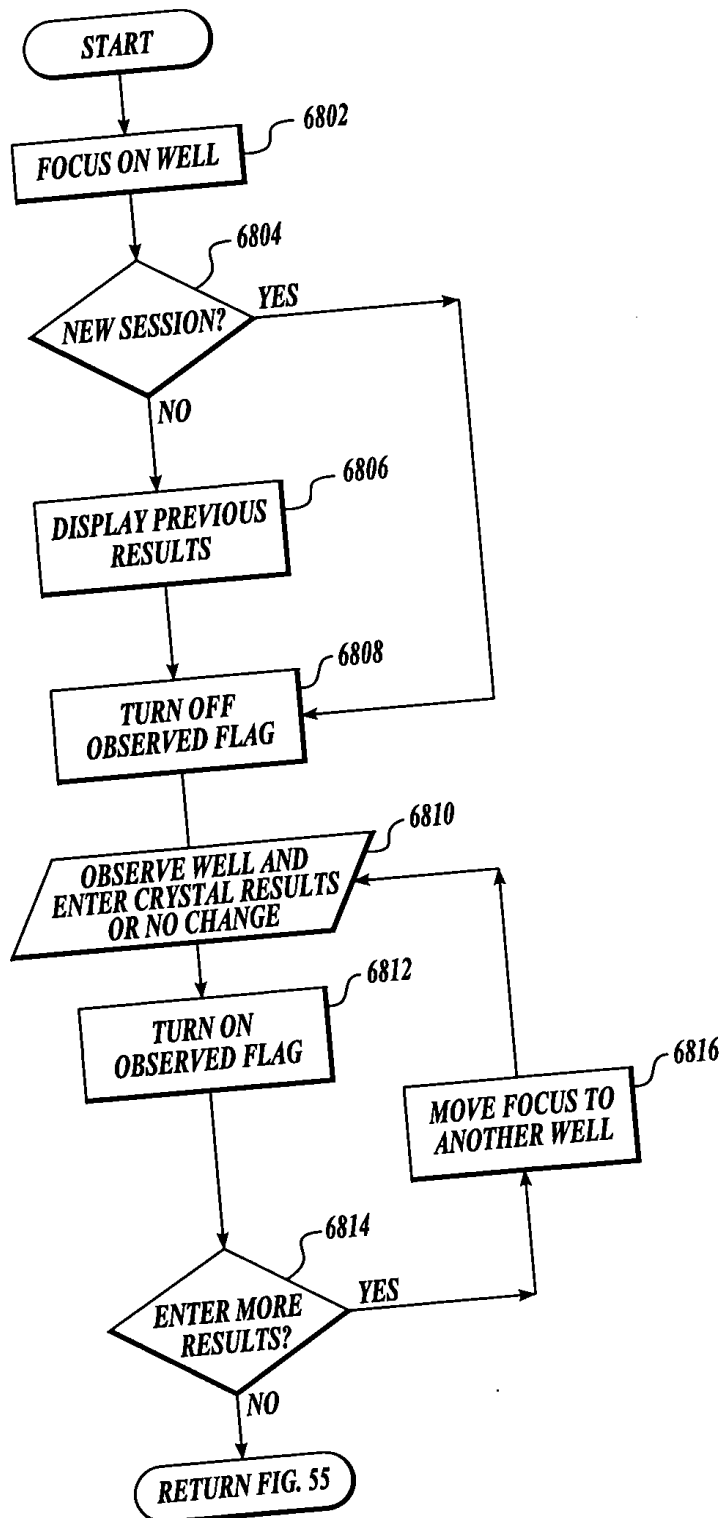
☒ Barcode Reader ON for Testing

Scanned Barcode:

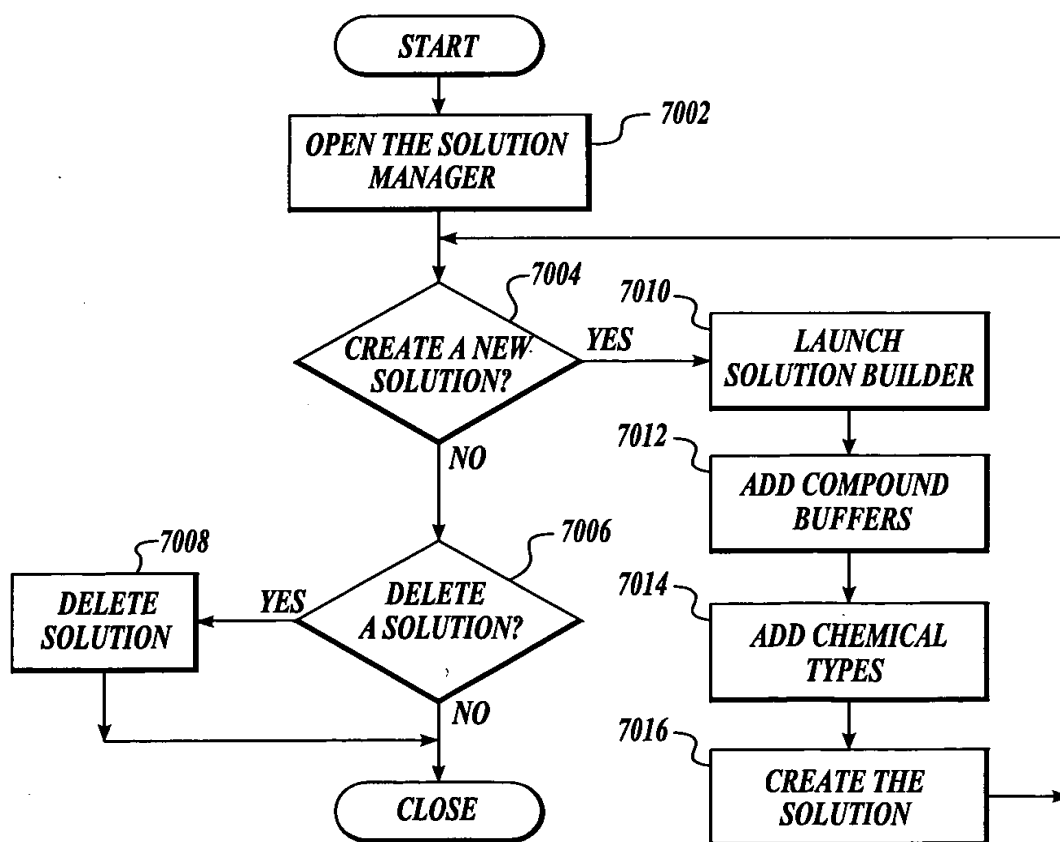
Set Defaults

OK Cancel

Fig. 67

*Fig. 68*

A1 clear	A2 clear	A3 clear	A4 clear	A5 ●pp+	A6 pp+
B1 ***	B2 clear	B3 clear	B4 clear	B5 clear	B6 ●
C1 △ =	C2 sph	C3 sph	C4 □	C5 □ □	C6 clear
D1 pp+	D2 pp+	D3 P	D4 P pp+	D5 clear	D6 pp+

Fig. 69*Fig. 70*

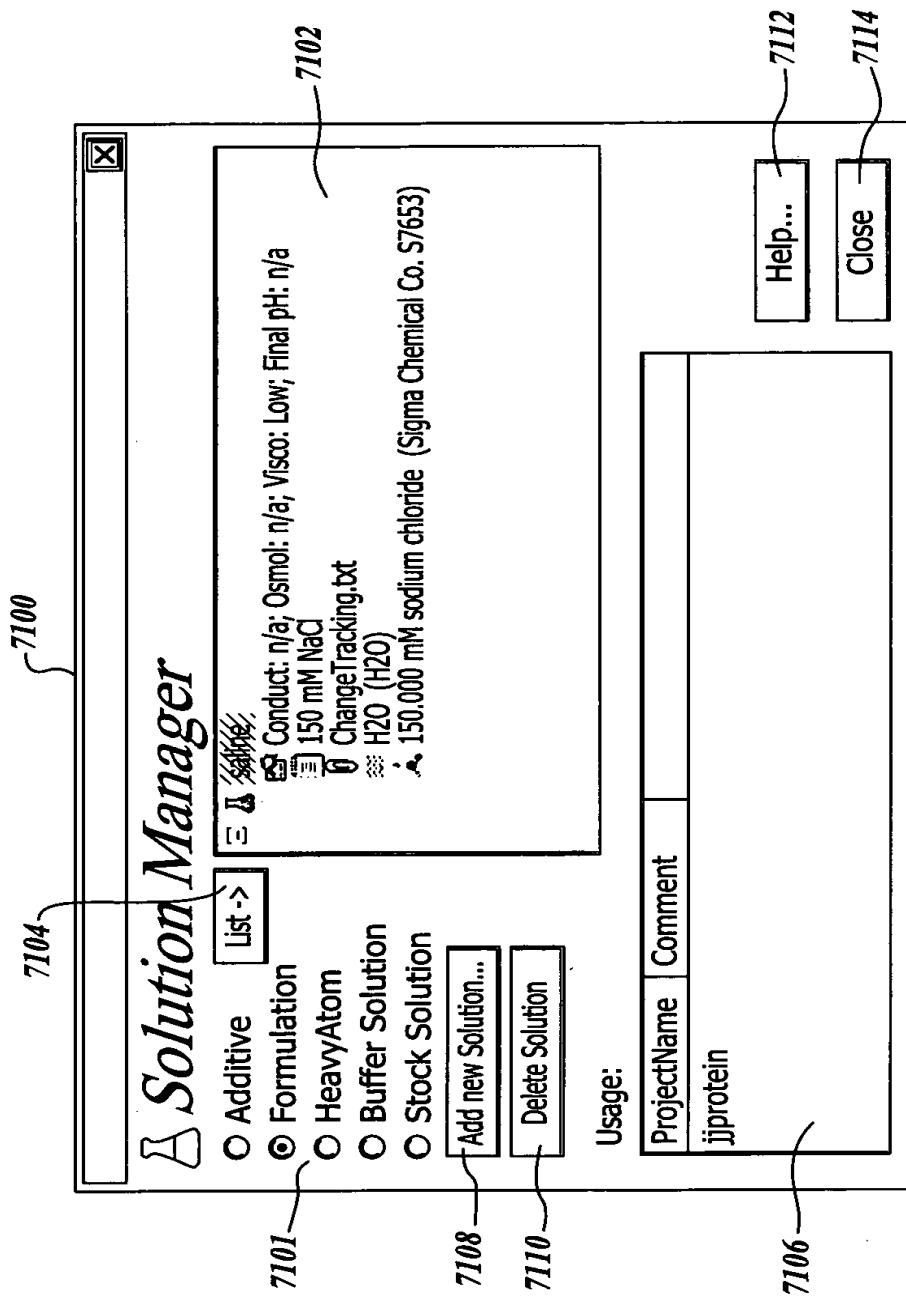
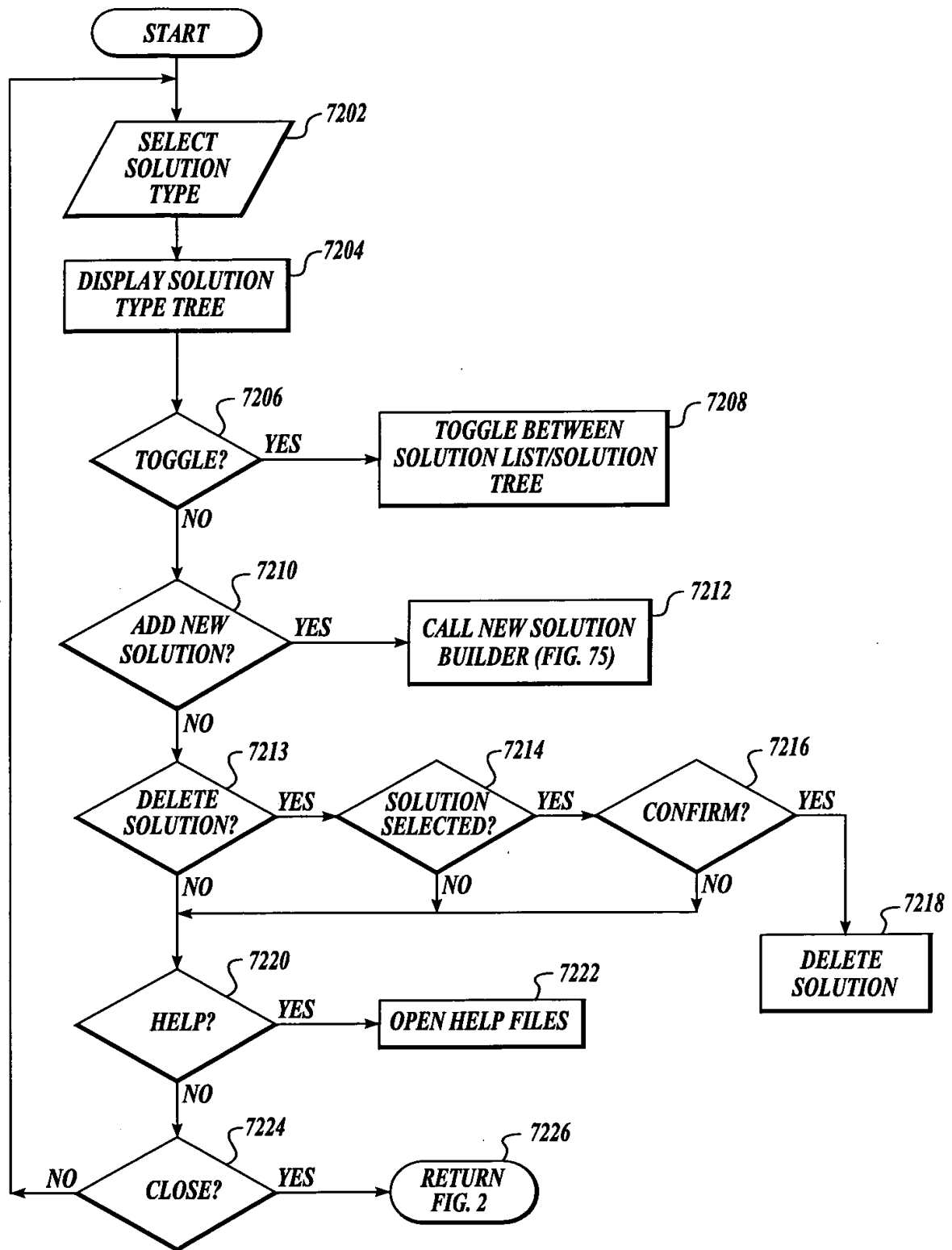
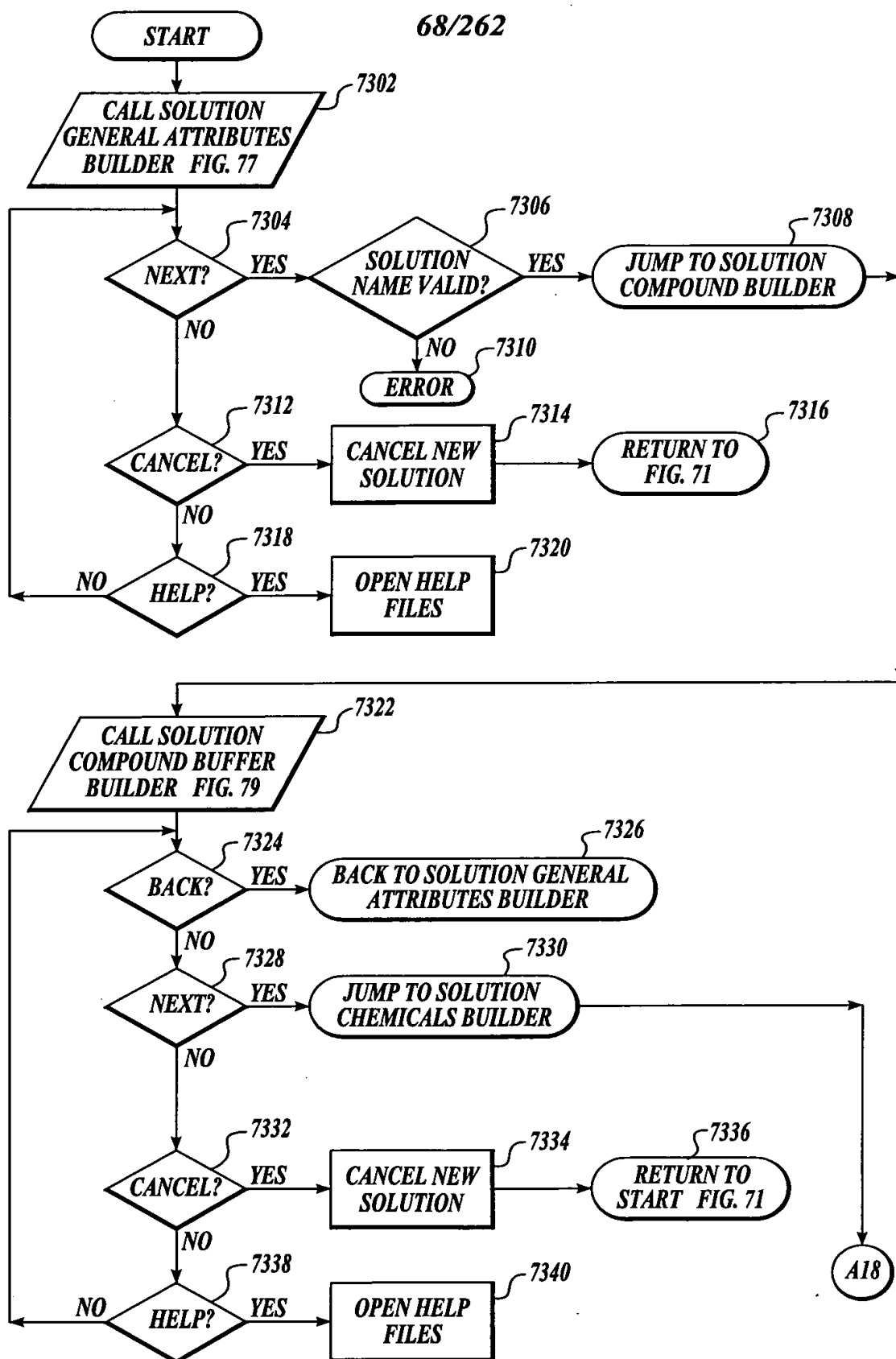
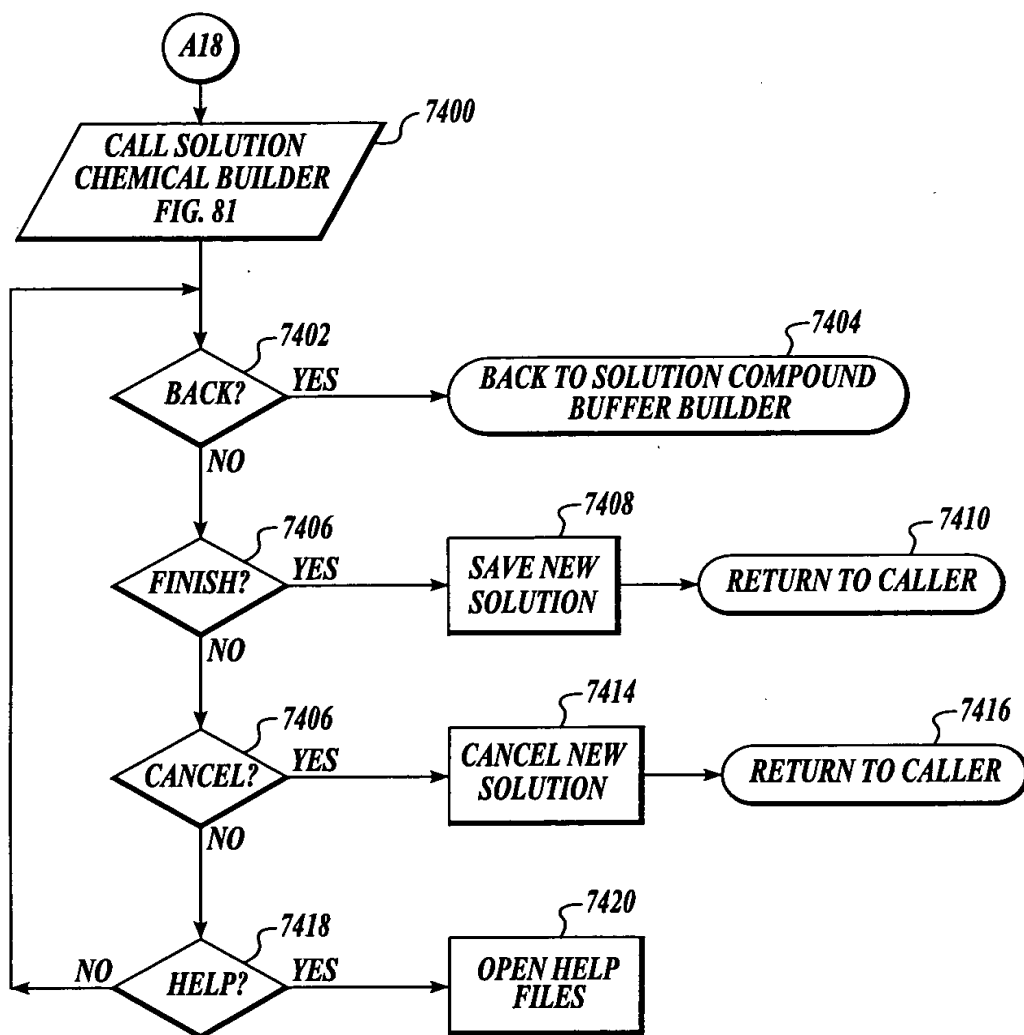


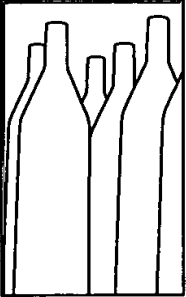
Fig. 71

*Fig. 72*

*Fig. 73*

*Fig. 74*

Solution Wizard - General



Solution Type

- ☐ Additive
- ☒ Formulation
- ☐ Heavy Atom
- ☐ Buffer Solution
- ☐ Stock Solution

pH of Solution

- ☒ Estimate
- ☐ Measured

Viscosity

- ☒ Low
- ☐ High

Solution Attributes


pH of Solution:

Vapor Pressure Osmolality: mmole/kg

Conductivity: uS/cm

Solvent: H2O (Mothe)

Solution Name: ammsulf040400

 E:\crymon\Help\crystalmonitor\images\attac

Comment:

200 mM ammonium sulfate 100mM Tris pH 7.0

Buttons: Back, Next >, Cancel, Help

Fig. 75

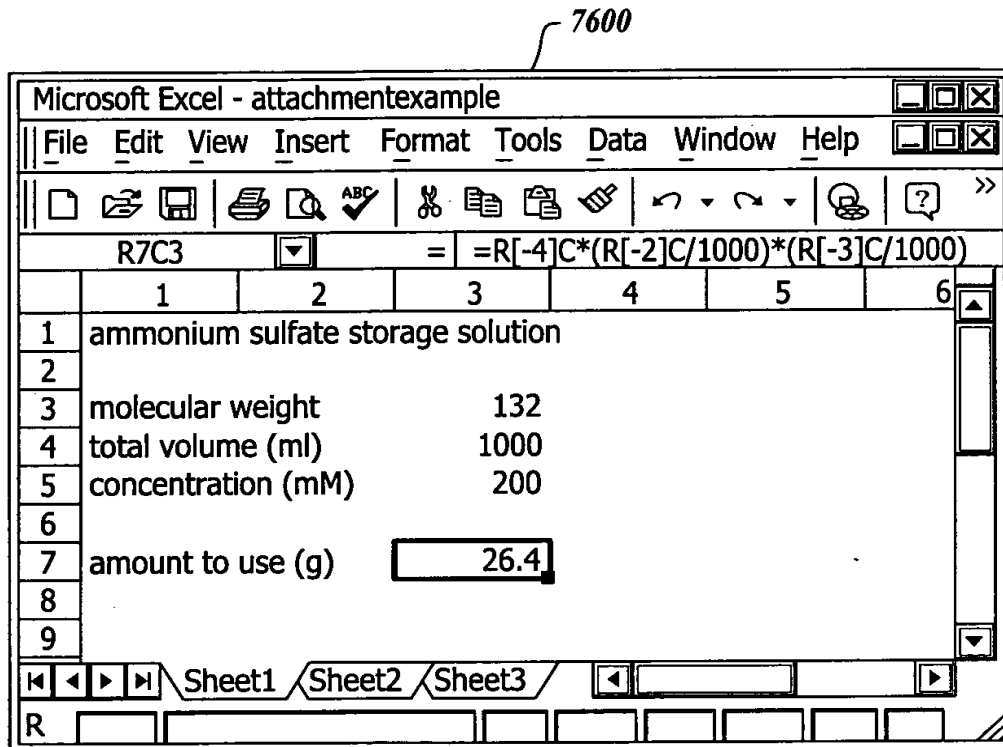
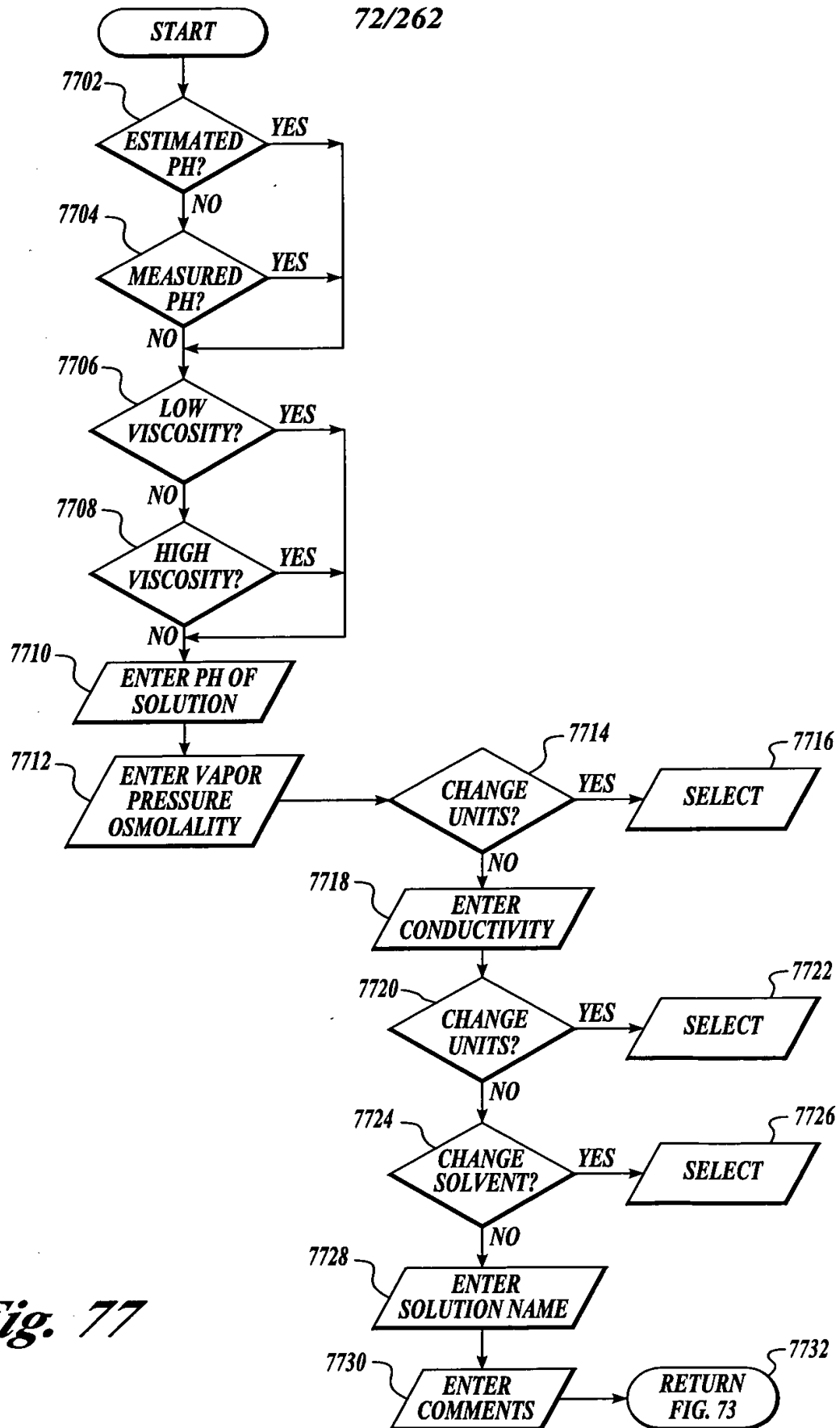


Fig. 76

*Fig. 77*

7800

Formulation: ammsulf040400

Compound Buffer Source List:

Buffer PH	Buffering Agent	pH Conjugate	Commer
6.50	sodium cacodylic acid trihydr...	hydrochloric acid (HCl)	Na cac
6.50	2-morpholinoethanesulfonic a...	sodium hydroxide (NaOH)	MES-N
7.00	1,3-diaza-2,4-cyclopentadien...	hydrochloric acid (HCl)	imidaz
7.00	sodium cacodylic acid trihydr...	hydrochloric acid (HCl)	Na cac
7.00	4-(2-hydroxyethyl)piperazine-1...	sodium hydroxide (NaOH)	HEPES
7.00	tris(hydroxymethyl)aminometh...	hydrochloric acid (HCl)	Tris-H
7.50	N-(2-hydroxyethyl)piperazine-...	sodium hydroxide (NaOH)	HEPES

7801

7804

7806

Add Remove

Solution Buffer List:

Buffer PH	Concentration	Buffering Agent	pH Conjugate	Commer
7.00	100.00mM	tris(hydroxymethyl)am...	hydrochloric acid (HCl)	Tris-HCl

7802

7808

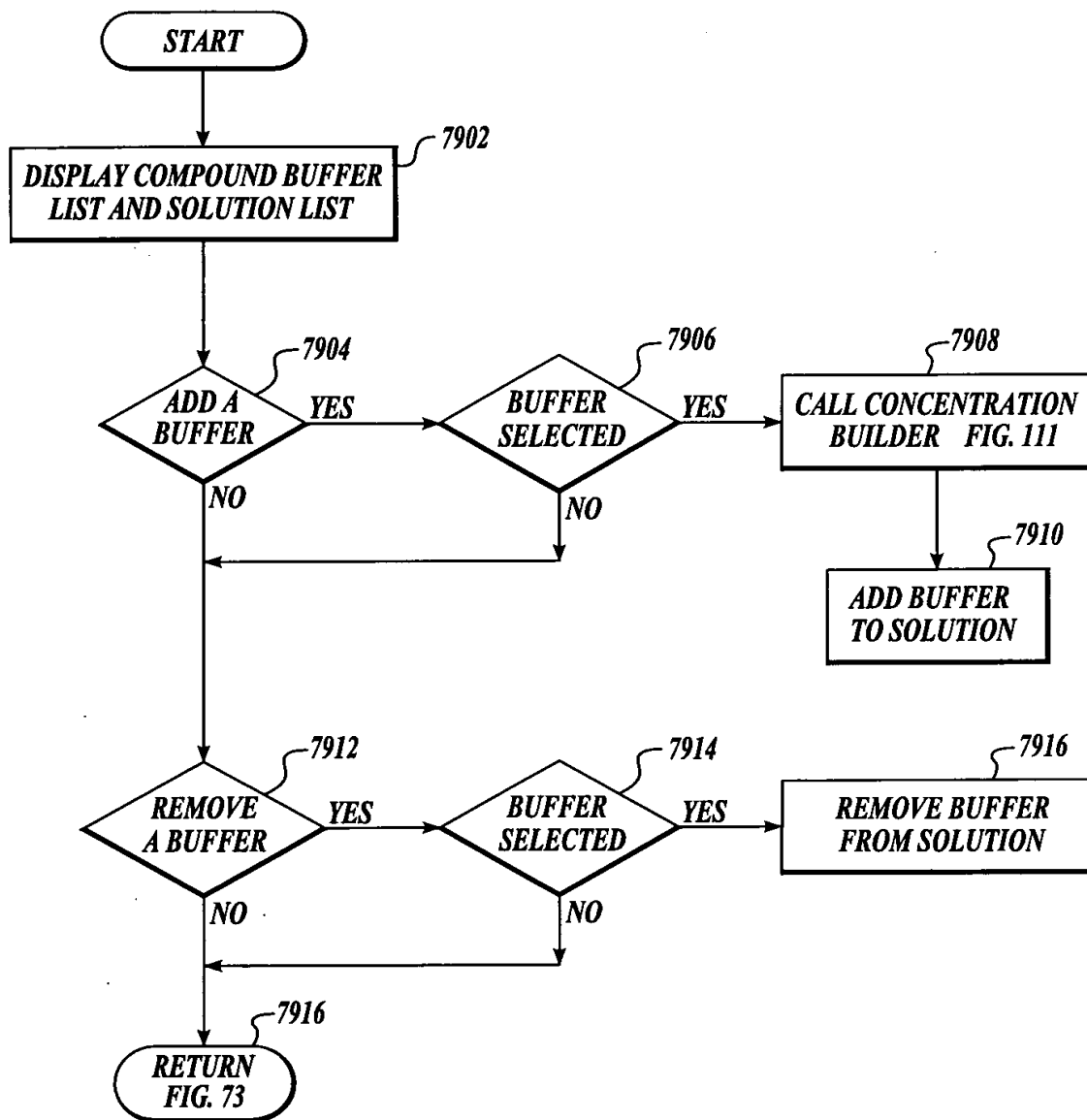
7810

7812

7814

Back Next > Cancel Help

Fig. 78

*Fig. 79*

8000

Formulation: ammsulf040400

New Chemical... 8004

Category:

- Buffer Agent
- Chelator
- CryoCoolant
- CSI
- Detergent
- Gas
- HeavyAtomCompound
- Metal
- NucleationSuppressant
- Organic
- Other
- pHConjugate
- Precipitant
- ReducingAgent
- Salt
- Solvent

Chemical Name

ammonium chloride (NH4 chloride)

ammonium dihydrogen phosphate (NH4 H2 phosp...

ammonium formate (NH3 formate)

ammonium nitrate (NH4 nitrate)

ammonium phosphate dibasic ((NH4)2 H phospha...

ammonium sulfate ((NH4)2 sulfate)

ammonium sulfate ((NH4)2 sulfate)

ammonium sulfate ((NH4)2 sulfate)

Formu

NH4C

NH4H

CH2O

NH4N

(NH4)

(NH4)

(NH4)

(NH4)

8002

8006

Delete Component

Solution Composition List:

Concentration	Chemical Name
200.000 mM	ammonium sulfate ((NH4)2 sulfate)

8003

<Back

Finish

Cancel

Help

8008

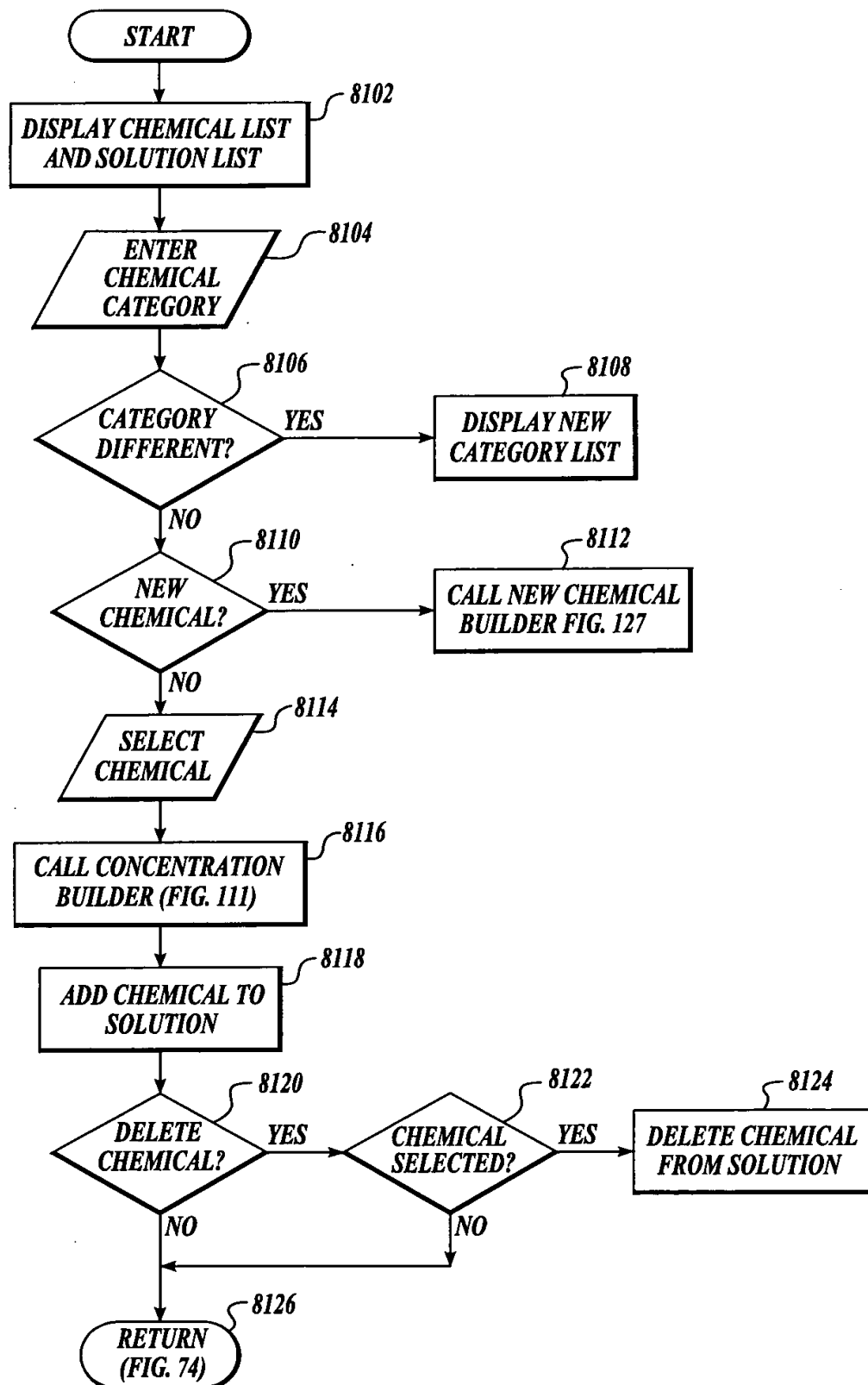
8010

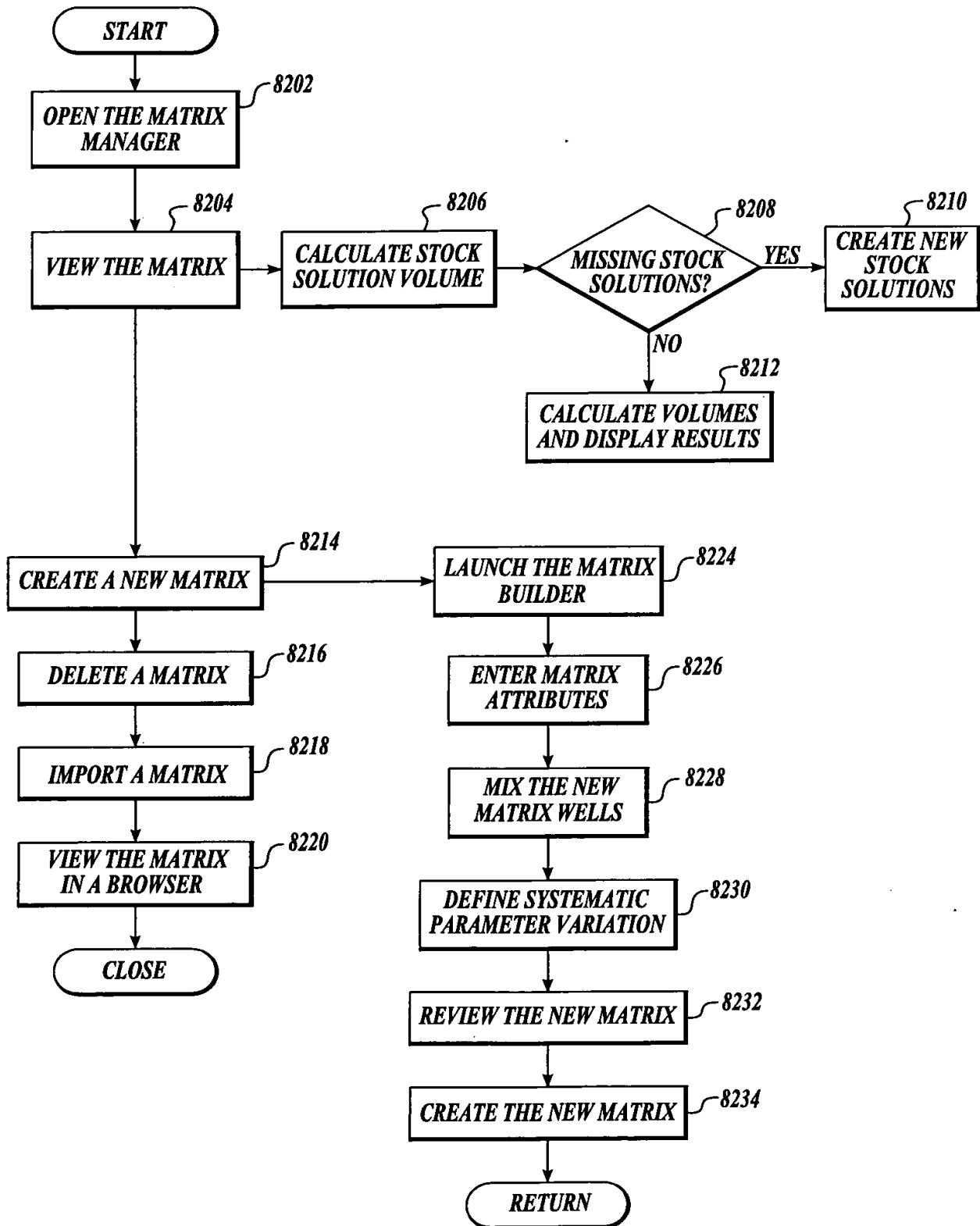
8012

8014

8001

Fig. 80

*Fig. 81*

*Fig. 82*

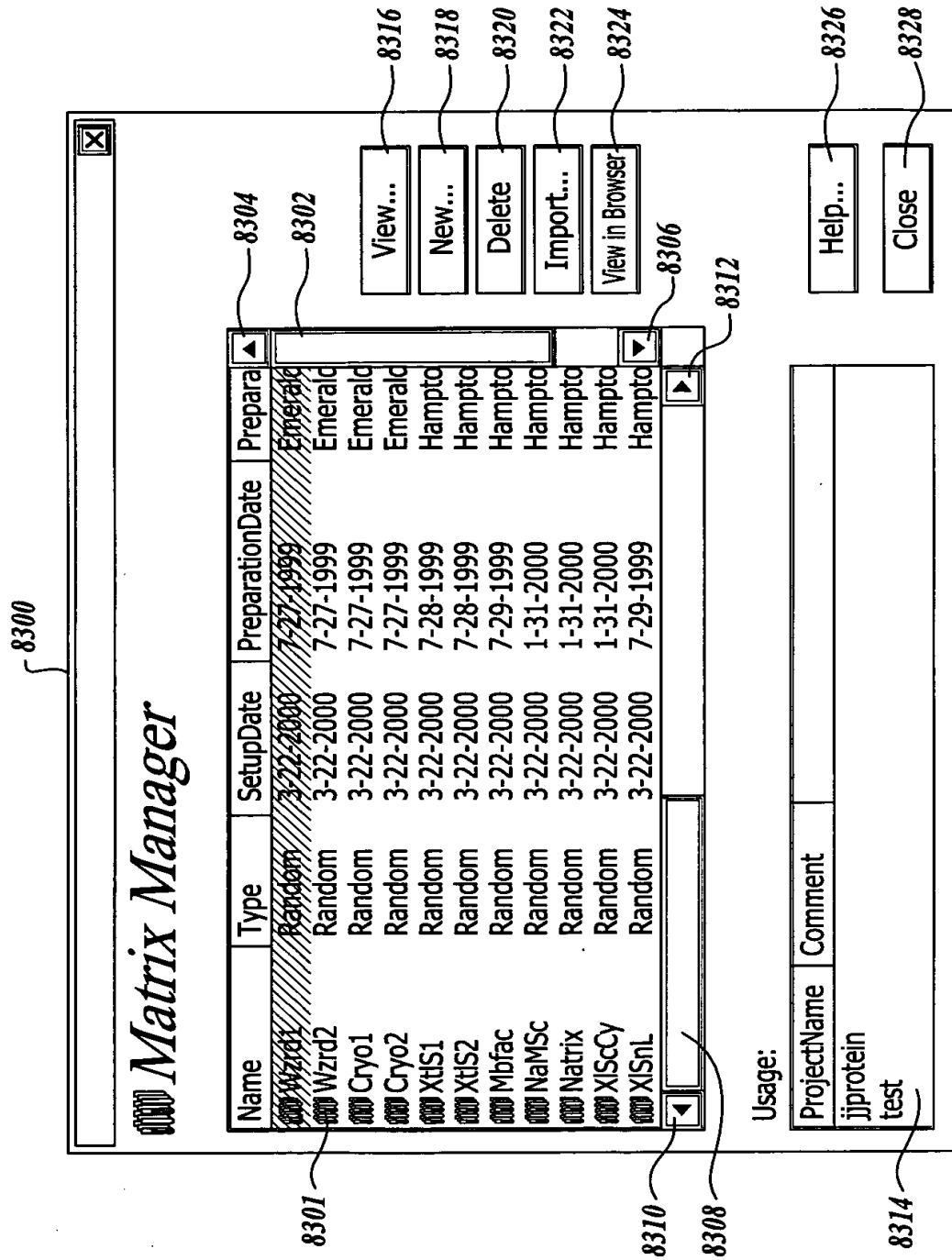
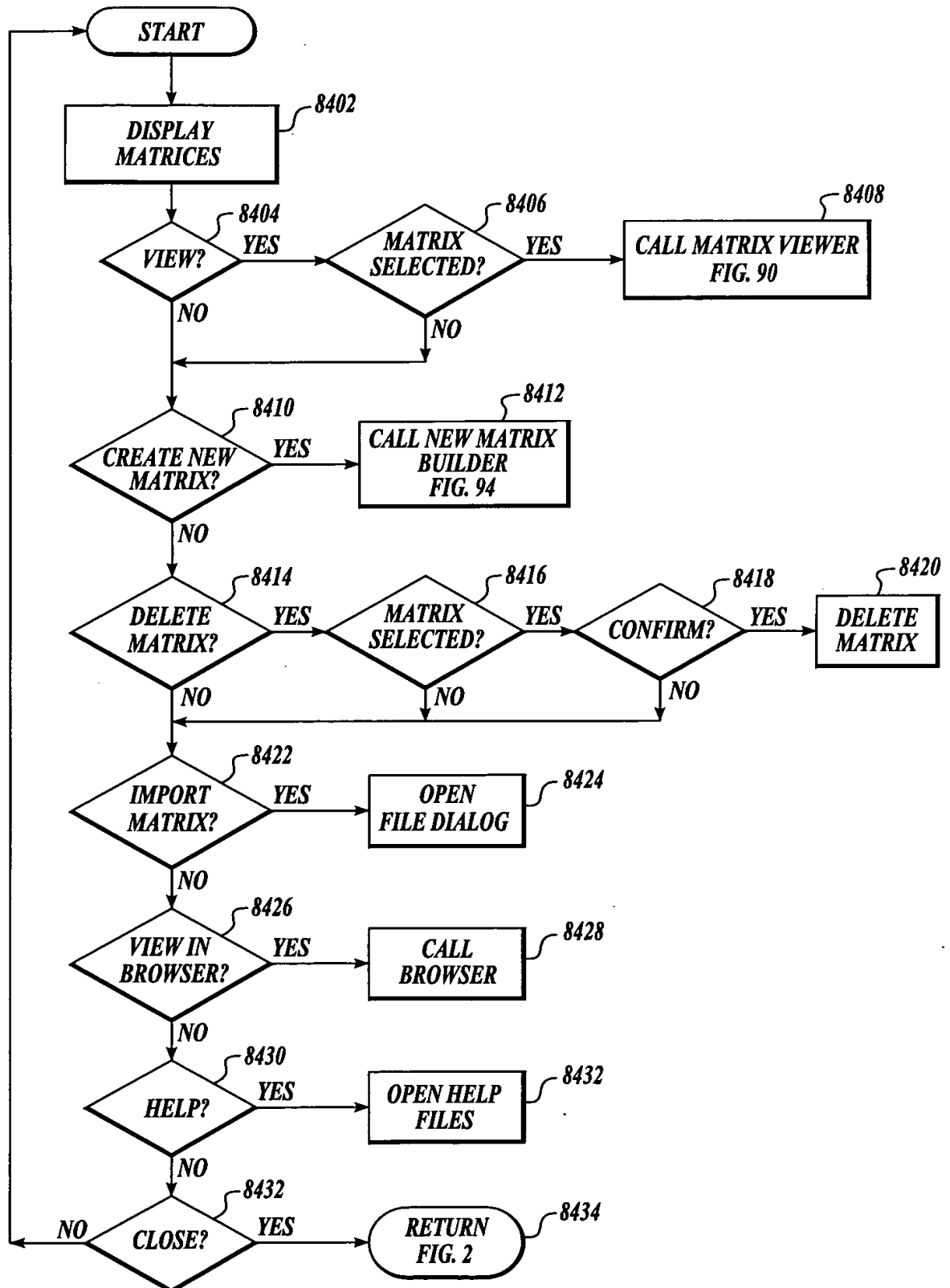


Fig. 83

*Fig. 84*

8500

Matrix Viewer

8501

(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)

8502

Matrix Name: newsys061599

Matrix Type: Systematic

Commercial: No

Preparator: Admin

X-Axis (systematically varied): polyethylene glycol 200

Y-Axis (systematically varied): sodium chloride

Comment:

8504

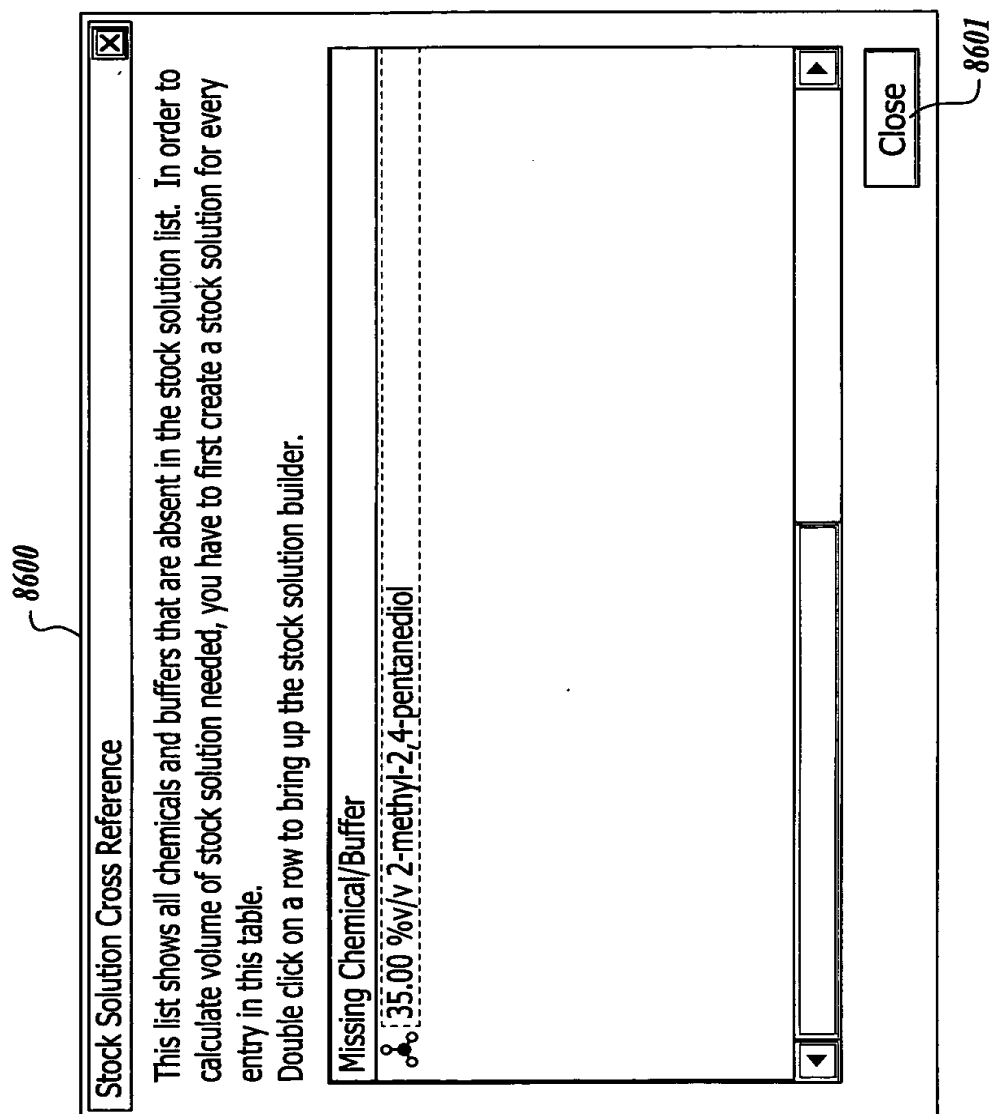
OK Cancel

8506

8502

Calc. Stock Sol. Vol. needed

Fig. 85

*Fig. 86*

8700

New Stock Solution (2-methyl-2,4-pentanediol) 8701

Solution Attributes

pH of Solution: 8702

Vapor Pressure Osmolality: mmole/kg 8706 8704

Conductivity: $\mu\text{S}/\text{cm}$ 8712

Solvent: H2O (Mothe) 8710 8714

Solution Name: MPD 100% (v/v) stock 8718

Concentration: 100 %v/v 8720 8722

pH of Solution

☐ Estimate 8726

☐ Measured

Viscosity

☒ Low 8728

☐ High

Comment:

100% (v/v) MPD stock 8730

Commit 8734 Cancel 8732

Fig. 87

Stock solution volumes to build matrix newsys061599

What is the final desired Crystallant volume?

10 ml

Calculate !

WellID	Volume	Stock Name	Stock Conc.	Chemical Name
1	1.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
1	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
1	8.800 ml		n/a	H2O
2	1.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
2	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
2	8.300 ml		n/a	H2O
3	2.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
3	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
3	7.800 ml		n/a	H2O
4	2.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
4	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...
4	7.300 ml		n/a	H2O
5	3.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...
5	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...

Close Help... View in Browser... Save to HTML...

Fig. 88

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WELLID	VOLUME	STOCK NAME	STOCK CONC.	CHEMICAL NAME	CHEMICAL TYPE	FINAL CONC.
1	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V CONC.
1	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM

Fig. 89A

1	8.800 ML		N/A	H ₂ O	SOLVENT	N/A
2	1.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	15.000 %V/V
2	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
2	8.300 ML		N/A	H ₂ O	SOLVENT	N/A
3	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
3	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
3	7.800 ML		N/A	H ₂ O	SOLVENT	N/A
4	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
4	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
4	7.300 ML		N/A	H ₂ O	SOLVENT	N/A
5	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
5	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
5	6.800 ML		N/A	H ₂ O	SOLVENT	N/A
6	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V

Fig. 89B

6	0.200 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	100.000 mM
6	6.300 ML		N/A	H2O	SOLVENT	N/A
7	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V
7	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
7	8.600 ML		N/A	H2O	SOLVENT	N/A
8	1.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	15.000 %V/V
8	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
8	8.100 ML		N/A	H2O	SOLVENT	N/A
9	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
9	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
9	7.600 ML		N/A	H2O	SOLVENT	N/A
10	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V

Fig. 89C

87/262

10	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
10	7.100 ML		N/A	H2O	SOLVENT	N/A
11	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
11	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
11	6.600 ML		N/A	H2O	SOLVENT	N/A
12	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V
12	0.400 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	200.000 mM
12	6.100 ML		N/A	H2O	SOLVENT	N/A
13	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V
13	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
13	8.400 ML		N/A	H2O	SOLVENT	N/A
14	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
14	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM

Fig. 89D

14	7.900 ML		N/A	H ₂ O	SOLVENT	N/A
15	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
15	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
15	7.400 ML		N/A	H ₂ O	SOLVENT	N/A
16	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
16	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
16	6.900 ML		N/A	H ₂ O	SOLVENT	N/A
17	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
17	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM
17	6.400 ML		N/A	H ₂ O	SOLVENT	N/A
18	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V
18	0.600 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	300.000 mM

Fig. 89E

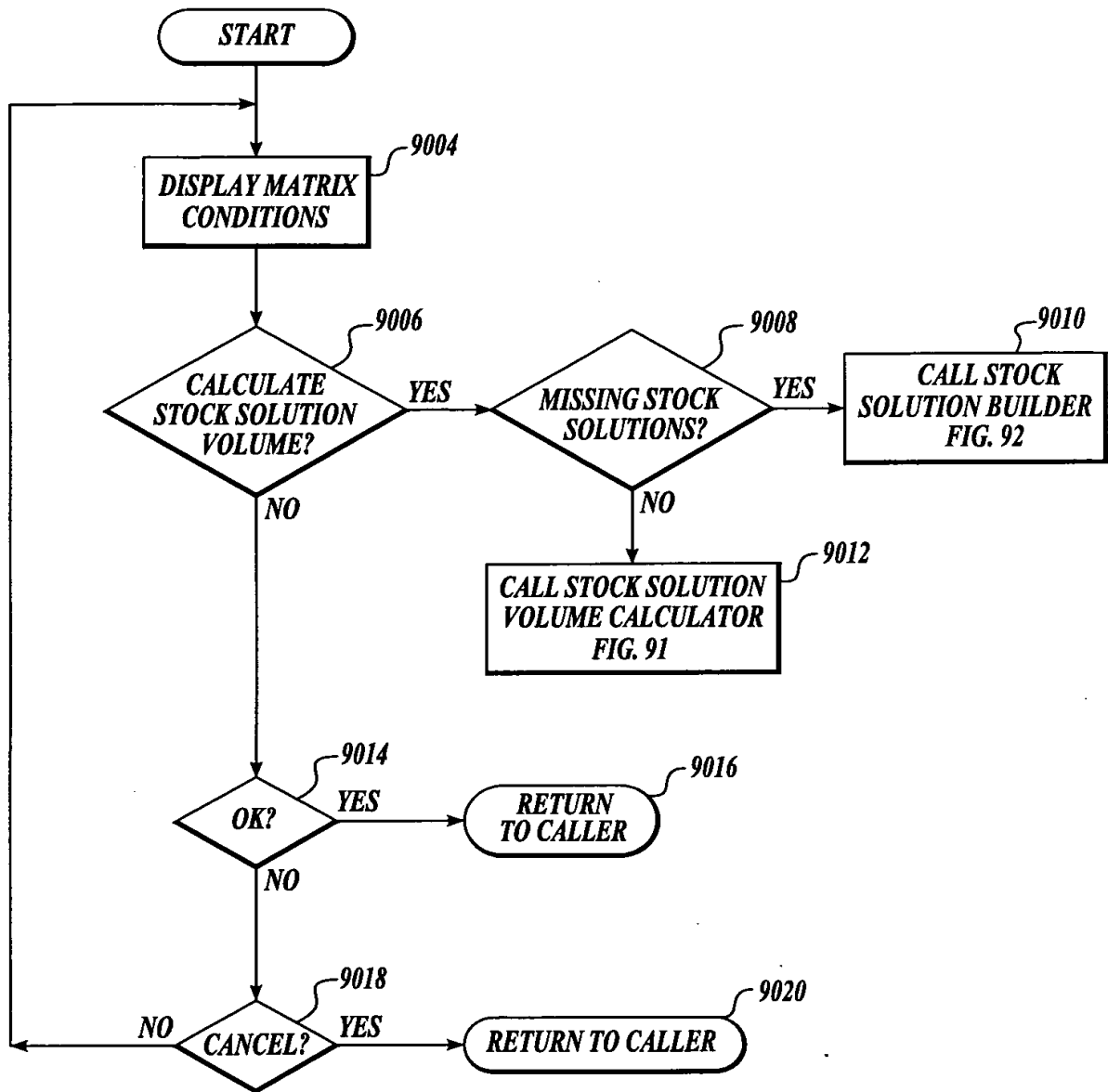
18	5.900 ML		N/A	H ₂ O	SOLVENT	N/A
19	1.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	10.000 %V/V
19	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
19	8.200 ML		N/A	H ₂ O	SOLVENT	N/A
20	1.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	15.000 %V/V
20	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
20	7.700 ML		N/A	H ₂ O	SOLVENT	N/A
21	2.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	20.000 %V/V
21	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
21	7.200 ML		N/A	H ₂ O	SOLVENT	N/A
22	2.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	25.000 %V/V
22	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM

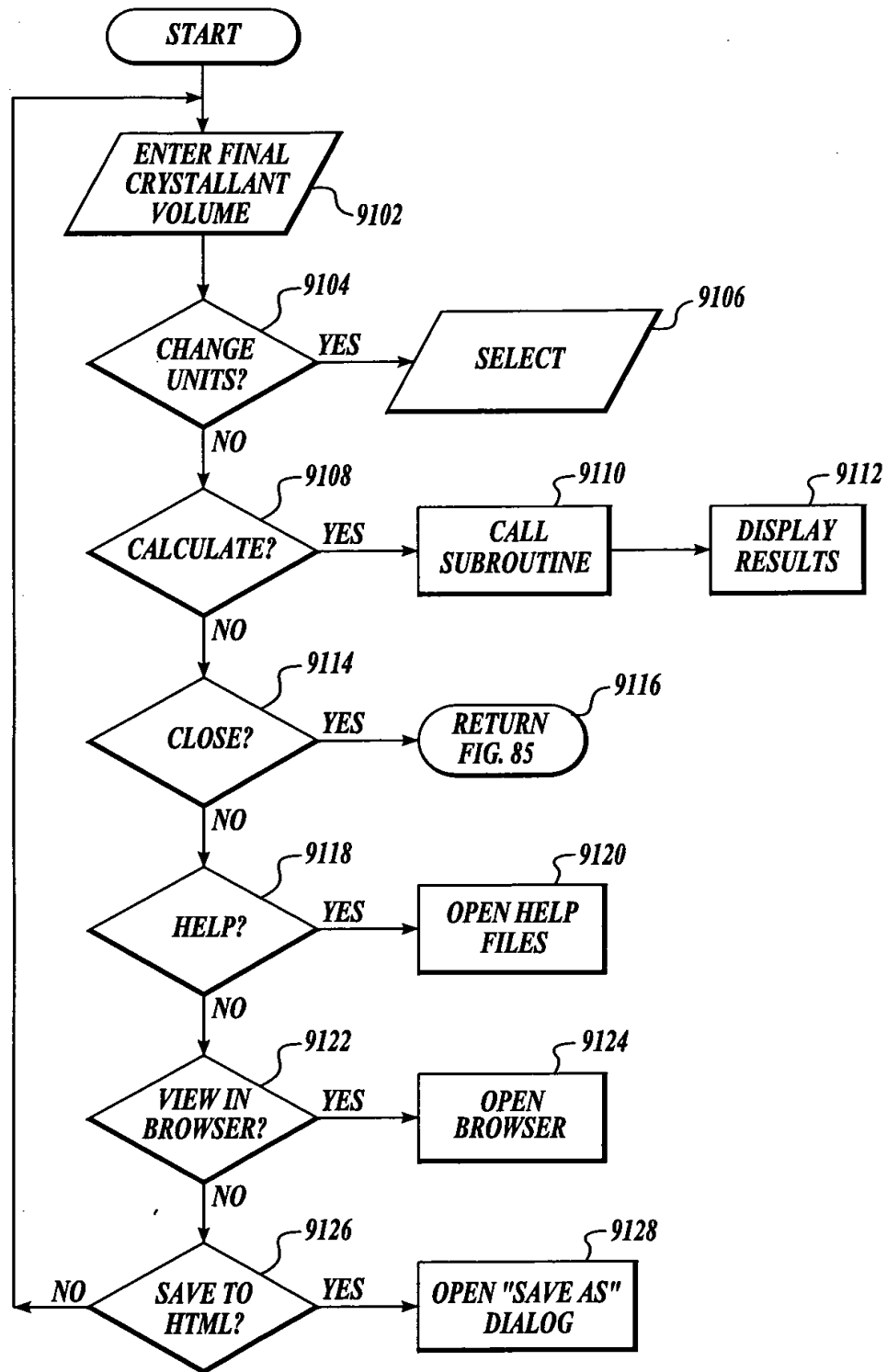
Fig. 89F

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22	6.700 ML		N/A	H2O	SOLVENT	N/A
23	3.000 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	30.000 %V/V
23	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
23	6.200 ML		N/A	H2O	SOLVENT	N/A
24	3.500 ML	PEG-200 STOCK	100.000 %V/V	PEG-200 (SIGMA CHEMICAL CO.)	PRECIPITANT	35.000 %V/V
24	0.800 ML	SODIUM CHLORIDE 5 M STOCK	5000.000 mM	SODIUM CHLORIDE (SIGMA CHEMICAL CO.)	PRECIPITANT	400.000 mM
24	5.700 ML		N/A	H2O	SOLVENT	N/A

Fig. 89G

*Fig. 90*

*Fig. 91*

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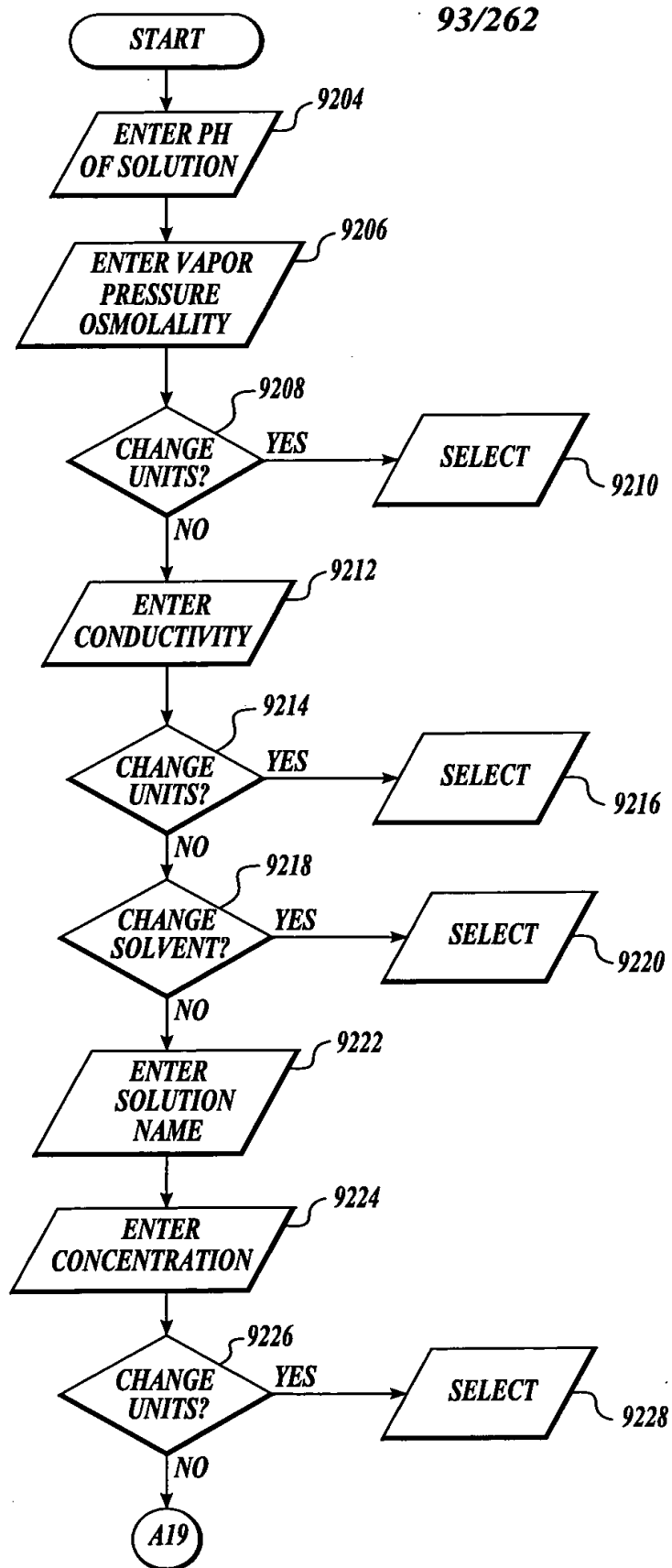
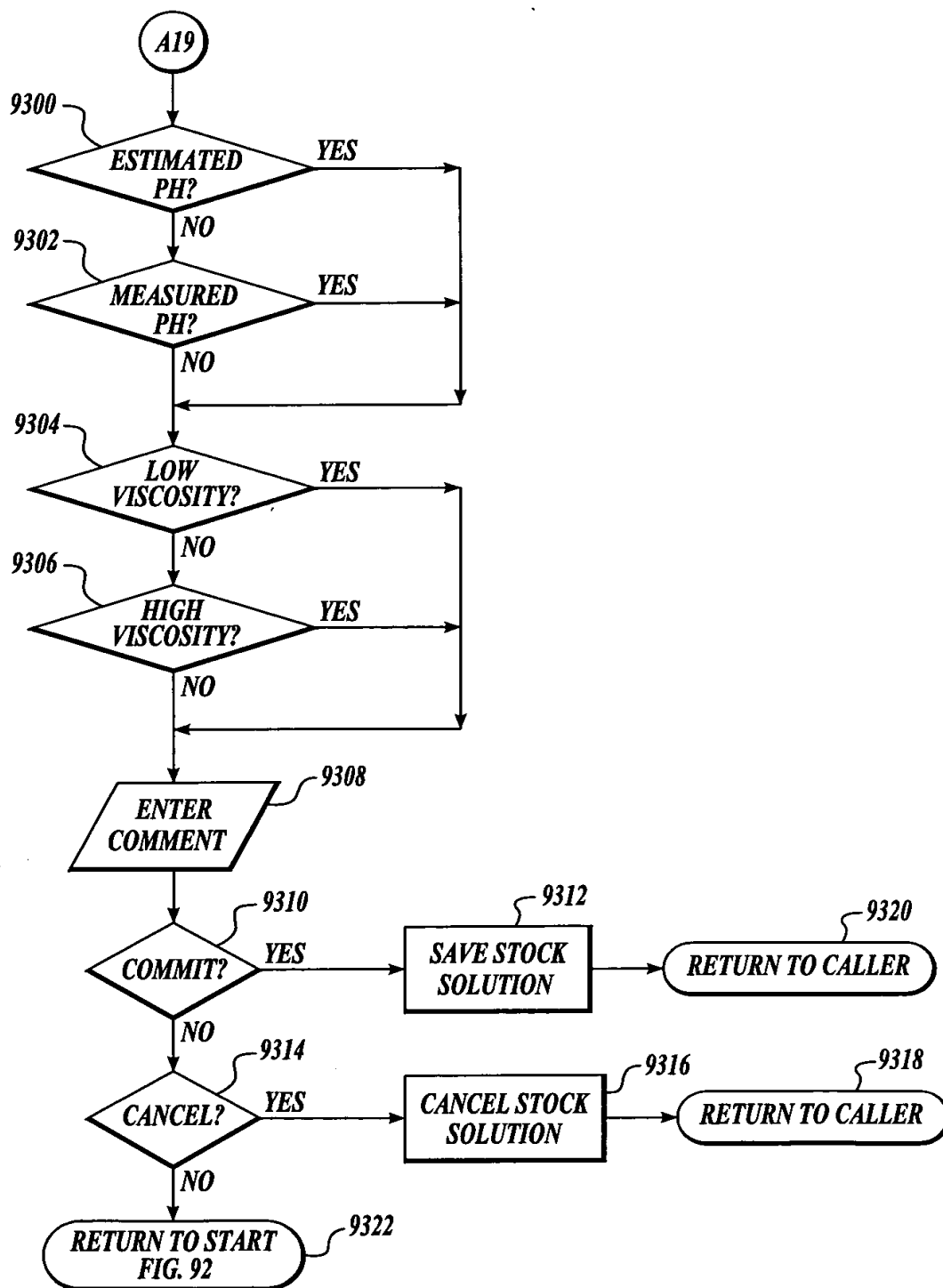
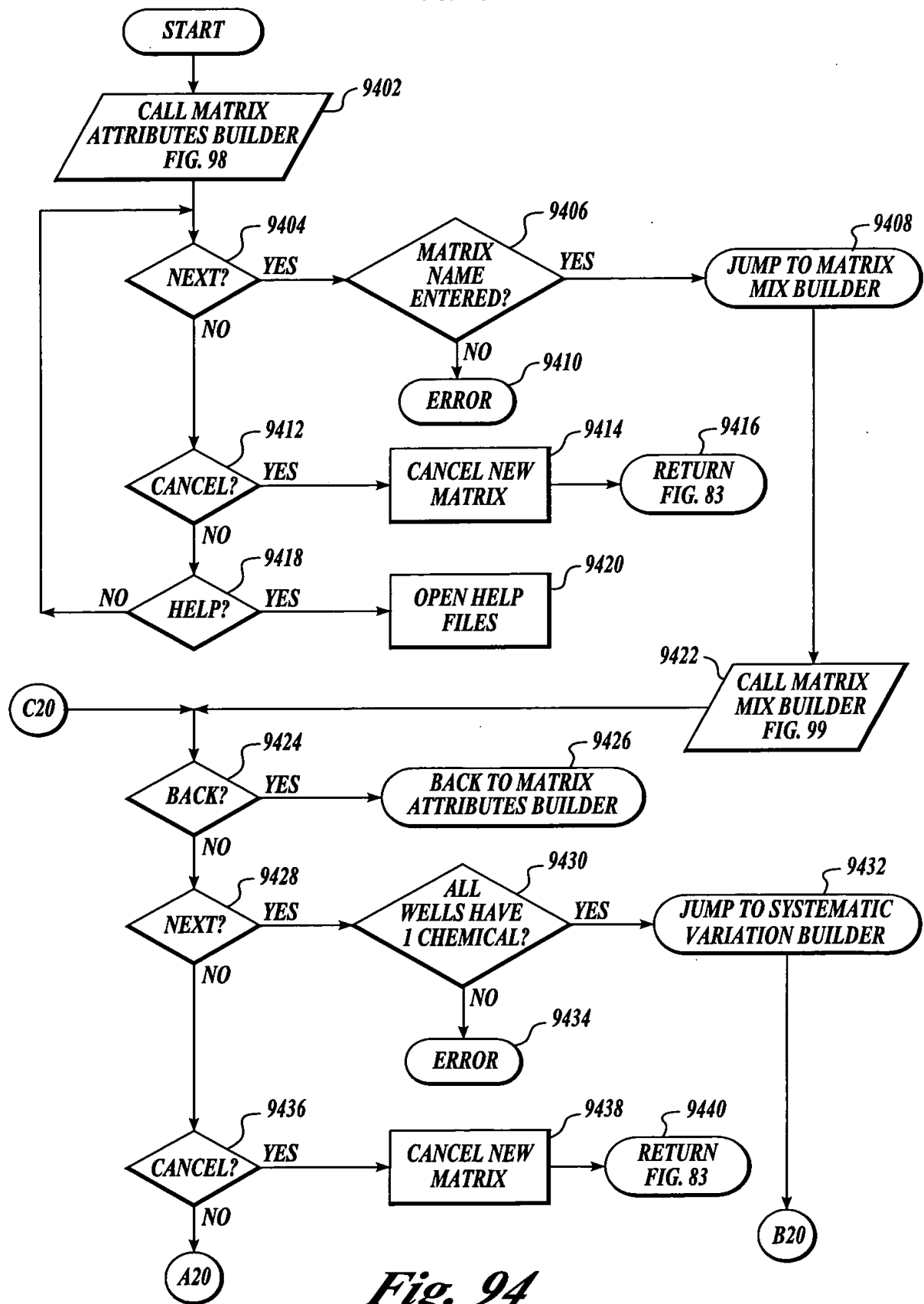
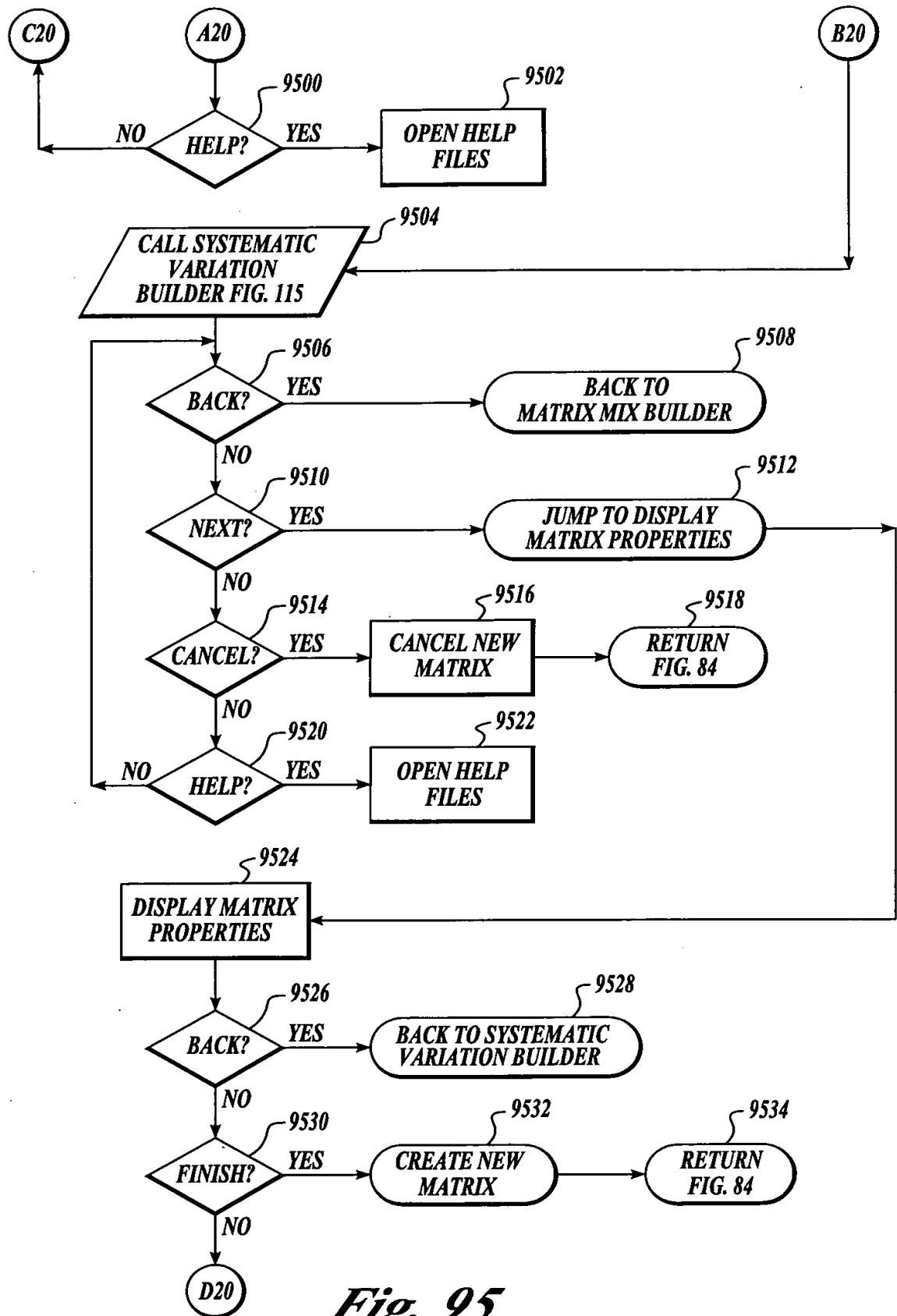
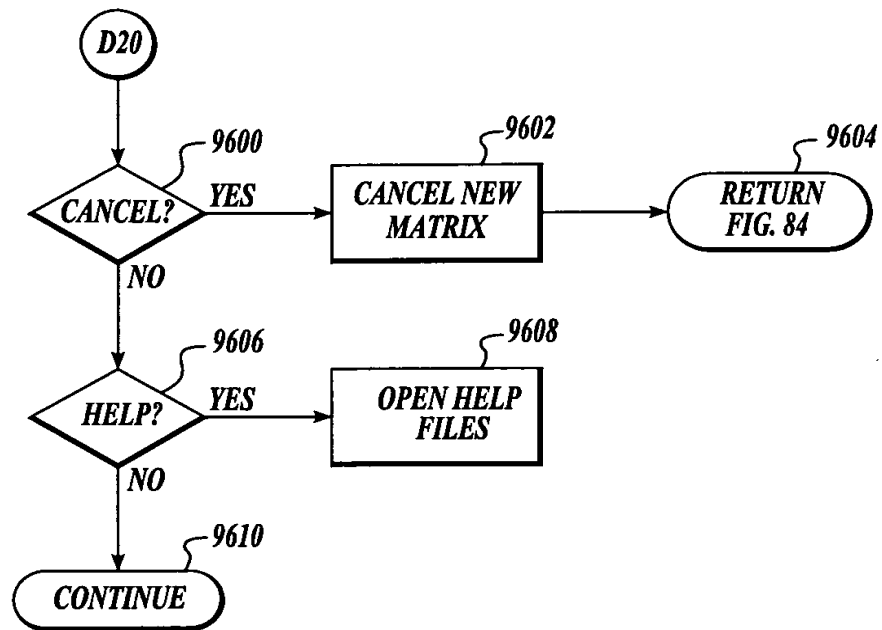


Fig. 92

*Fig. 93*



*Fig. 95*

*Fig. 96*

9700

9704, 9706

Matrix Wizard

Matrix Name: new48040400 9701

Well Count: 48 9702

Column Count: 6 9708

9710, 9712

Creator 9714

☒ Commercial (Matrix is available from a commercial source)

Preparator: Admin 9718

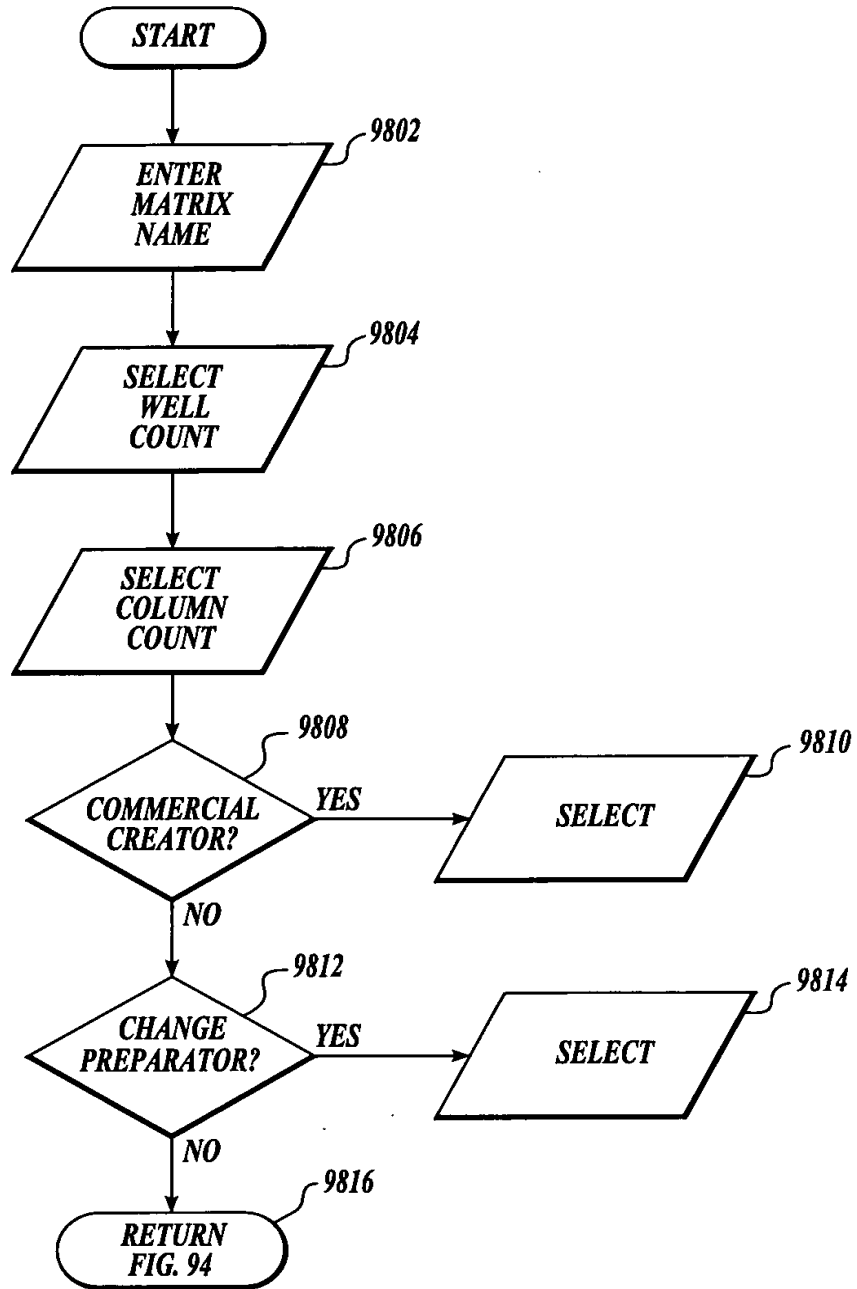
9716

Back Next > Cancel Help

9720 9722 9724 9726

The image shows a 'Matrix Wizard' dialog box. On the left is a grayscale image of a plant matrix. To the right are input fields for 'Matrix Name' (containing 'new48040400'), 'Well Count' (containing '48'), and 'Column Count' (containing '6'). Each of these fields has a small navigation icon to its left. Below these is a 'Creator' label and a checkbox labeled 'Commercial (Matrix is available from a commercial source)' which is checked. Underneath is a 'Preparator' label and a dropdown menu showing 'Admin'. At the bottom are four buttons: 'Back', 'Next >', 'Cancel', and 'Help'. Various reference numerals (9700, 9701, 9702, 9704, 9706, 9708, 9710, 9712, 9714, 9716, 9718, 9720, 9722, 9724, 9726) are connected by lines to specific UI elements.

Fig. 97

*Fig. 98*

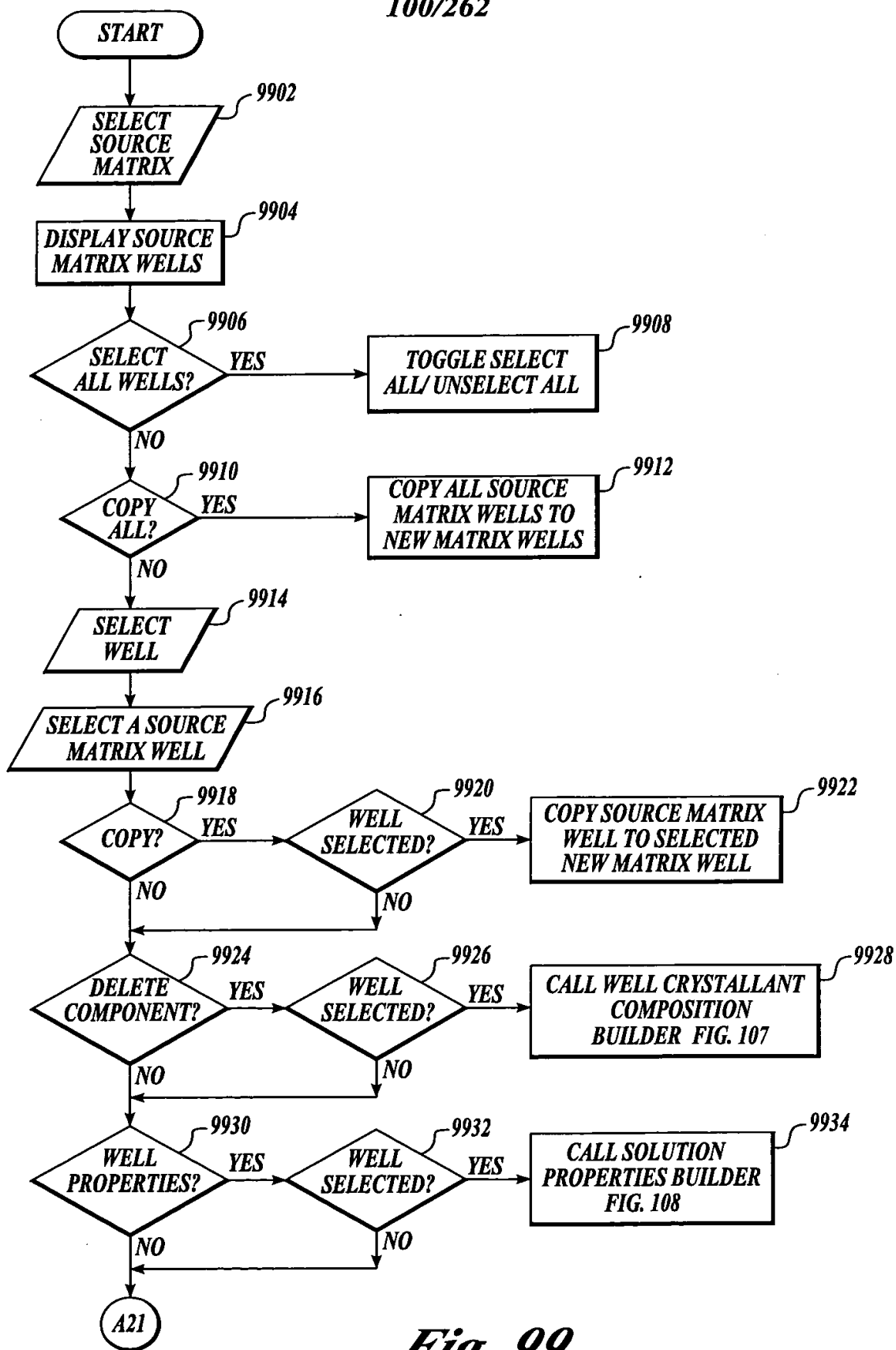


Fig. 99

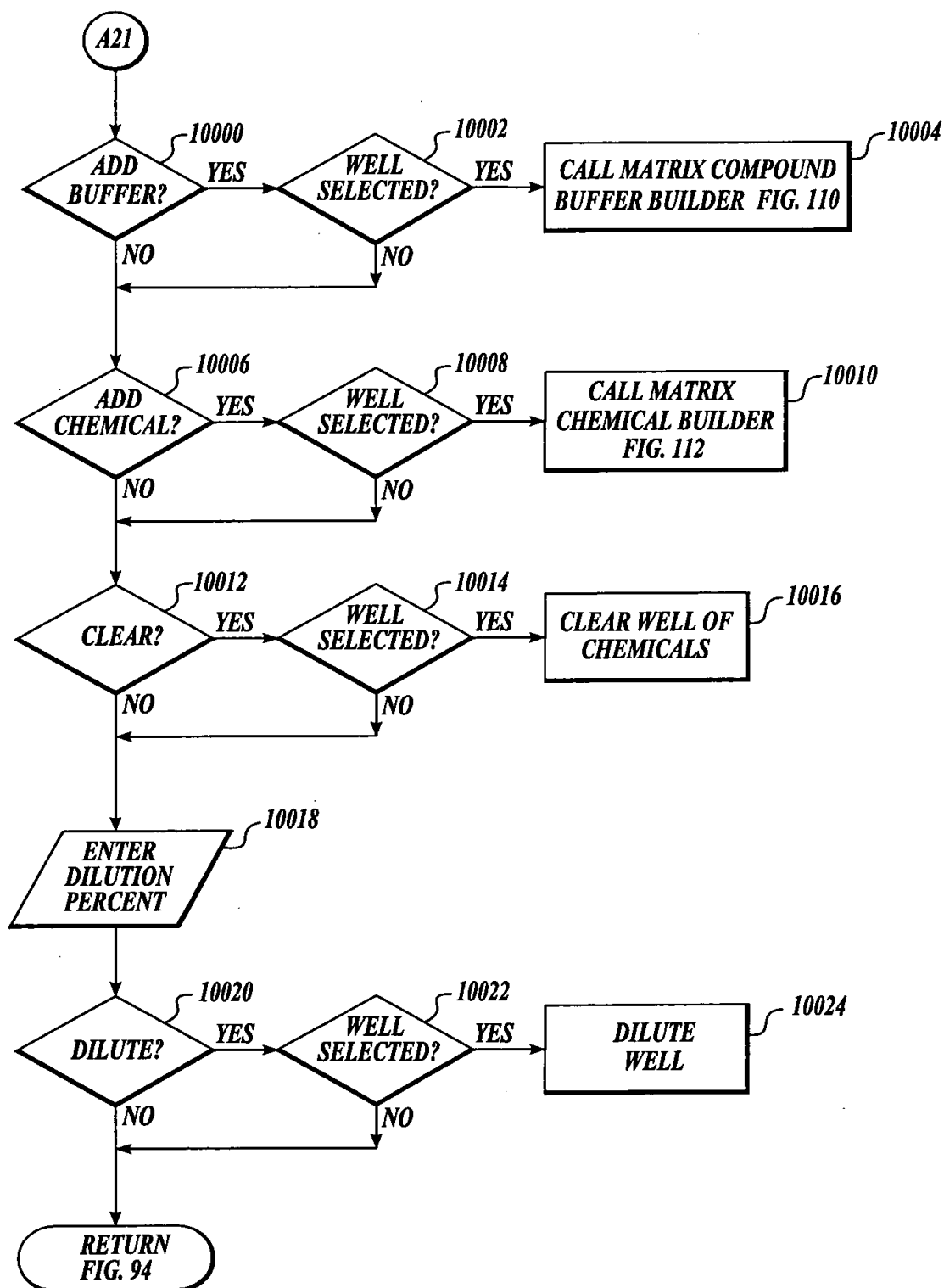
*Fig. 100*

Fig. 101

Matrix Wizard - Mix the new matrix

Select Source Matrix:

Cryo1 (48 conditions)

(2) pH 4.20	(2) pH 4.50	(2) pH 5.50	(3) pH 7.50	(3) pH 5.50	(3) pH 6.50
(3) pH 8.50	(2) pH 6.50	(2) pH 4.20	(2) pH 8.00	(3) pH 8.50	(3) pH 4.50
(3) pH 6.00	(4) pH 4.20	(3) pH 9.50	(4) pH 6.00	(2) pH 7.50	(3) pH 8.00
(2) pH 8.50	(3) pH 5.50	(3) pH 4.50	(2) pH 6.20	(3) pH 7.00	(3) pH 6.20
(3) pH 8.50	(3) pH 9.50	(4) pH 10.50	(4) pH 7.50	(3) pH 9.50	(2) pH 5.50
(3) pH 5.50	(3) pH 9.50	(4) pH 8.00	(3) pH 8.00	(3) pH 7.50	(3) pH 7.00

Emerald's Cryo 1 Crystal Growth Matrix. All crystallants (1-48) flash-freeze as an amorphous glass at 100K.

Clear Sel all... 1 Copy Copy all

Add Chem... Add Buffer... Properties... Del Comp...

(2) pH 4.20 (2) pH 4.20 (2) pH 4.20 (2) pH 4.20

-Well 1-

Compound Buffers:
50.000 mM (Na2 H phosphate, citric acid) pH 4.20

Chemicals:
20.000 %v/v MPD, Precipitant (Fluka Chemical Corp. 68340)

Solution Properties:
Final pH: 4.20 est.
Conductivity: n/a
Vapor Pressure Osmolality: n/a
Viscosity: Low
Solvent: H2O

< Back Next > Cancel Help

Fig. 102

10300

Crystallant Composition - Removal List

Check the box for the Chemicals to remove from the selected wells:

Chemical Name	Abbreviation	Formula
<input type="checkbox"/> 2-methyl-2,4-pentanediol	MPD	C ₆ H ₁₄ O ₂

10304a

10301

Check the box for the Compound Buffers to remove from the selected wells:

Buffer PH	Buffering Agent	pH Conjugate
<input type="checkbox"/> 4.20	sodium phosphate dibasic (N...	citric acid monohydrate (citric...

10304b

10302

OK Cancel

10306 10308

Fig. 103

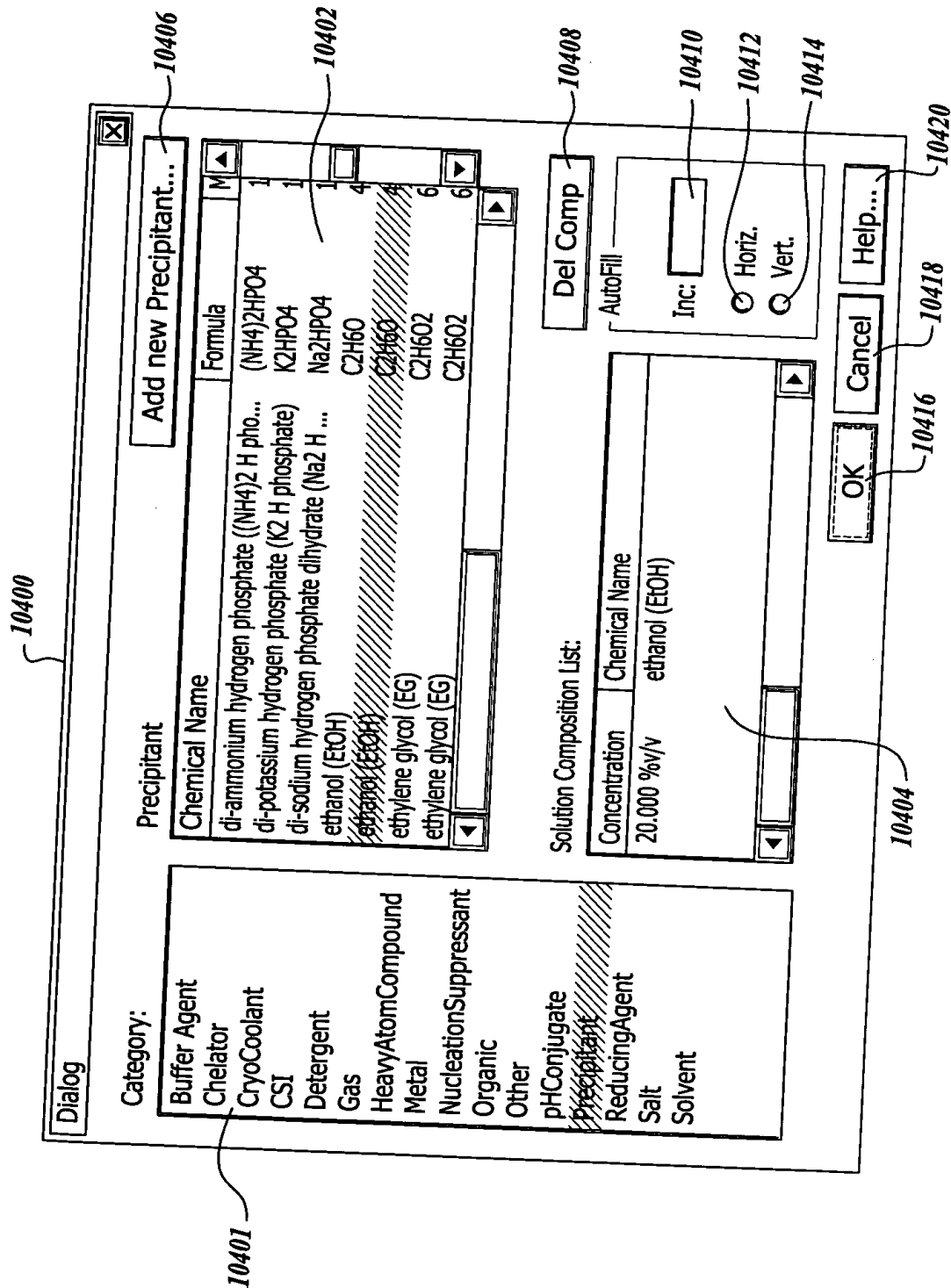


Fig. 104

Dialog

Add new Precipitant...

Category:

- Buffer Agent
- Chelator
- CryoCoolant
- CSI
- Detergent
- Gas
- HeavyAtomCompound
- Metal
- NucleationSuppressant
- Organic
- Other
- pHConjugate
- ~~Precipitant~~
- ReducingAgent
- Salt
- Solvent

Precipitant

Chemical Name	Formula	M
polyethylene glycol 12000 (PEG-12000)	H(OCH ₂ CH ₂ O)nH	1
polyethylene glycol 1500 (PEG-1500)	H(OCH ₂ CH ₂ O)nH	1
polyethylene glycol 1500 (PEG-1500)	H(OCH ₂ CH ₂ O)nH	1
polyethylene glycol 200 (PEG-200)	H(OCH ₂ CH ₂ O)nH	2
polyethylene glycol 200 (PEG-200)	H(OCH ₂ CH ₂ O)nH	2
polyethylene glycol 200 (PEG-200)	H(OCH ₂ CH ₂ O)nH	2
polyethylene glycol 2000 dimethyl ether (PEG-2000...)	H(OCH ₂ CH ₂ O)nH	2

Solution Composition List:

Concentration	Chemical Name
10.000 %v/v	polyethylene glycol 200 (PEG-200)

Del Comp

AutoFill

Inc: 10500

☒ Horiz. 10502

☐ Vert.

OK Cancel Help...

Fig. 105

10600

Matrix Wizard - Mix the new matrix

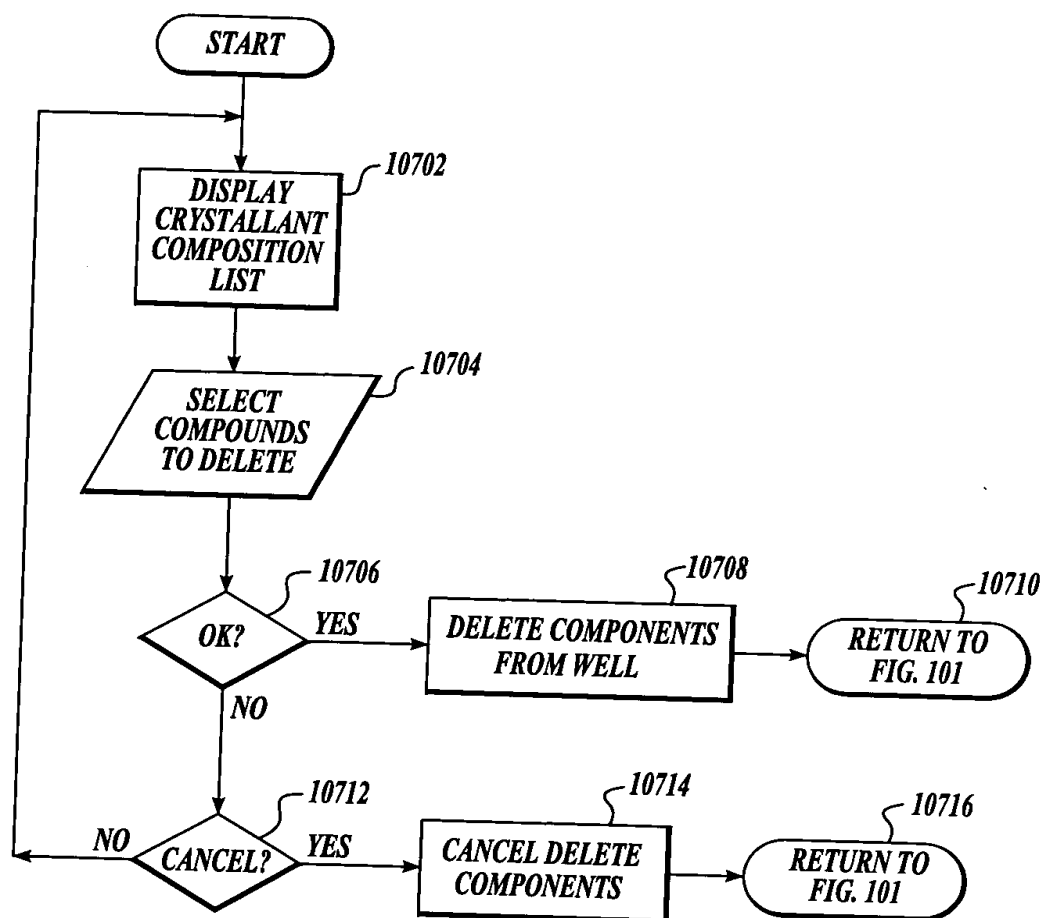
Select Source Matrix: Dilution(%) Dilute sel.

<Select Matrix>

(1)	(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)	(1)

<Back Next > Cancel Help

Fig. 106

*Fig. 107*

109/262

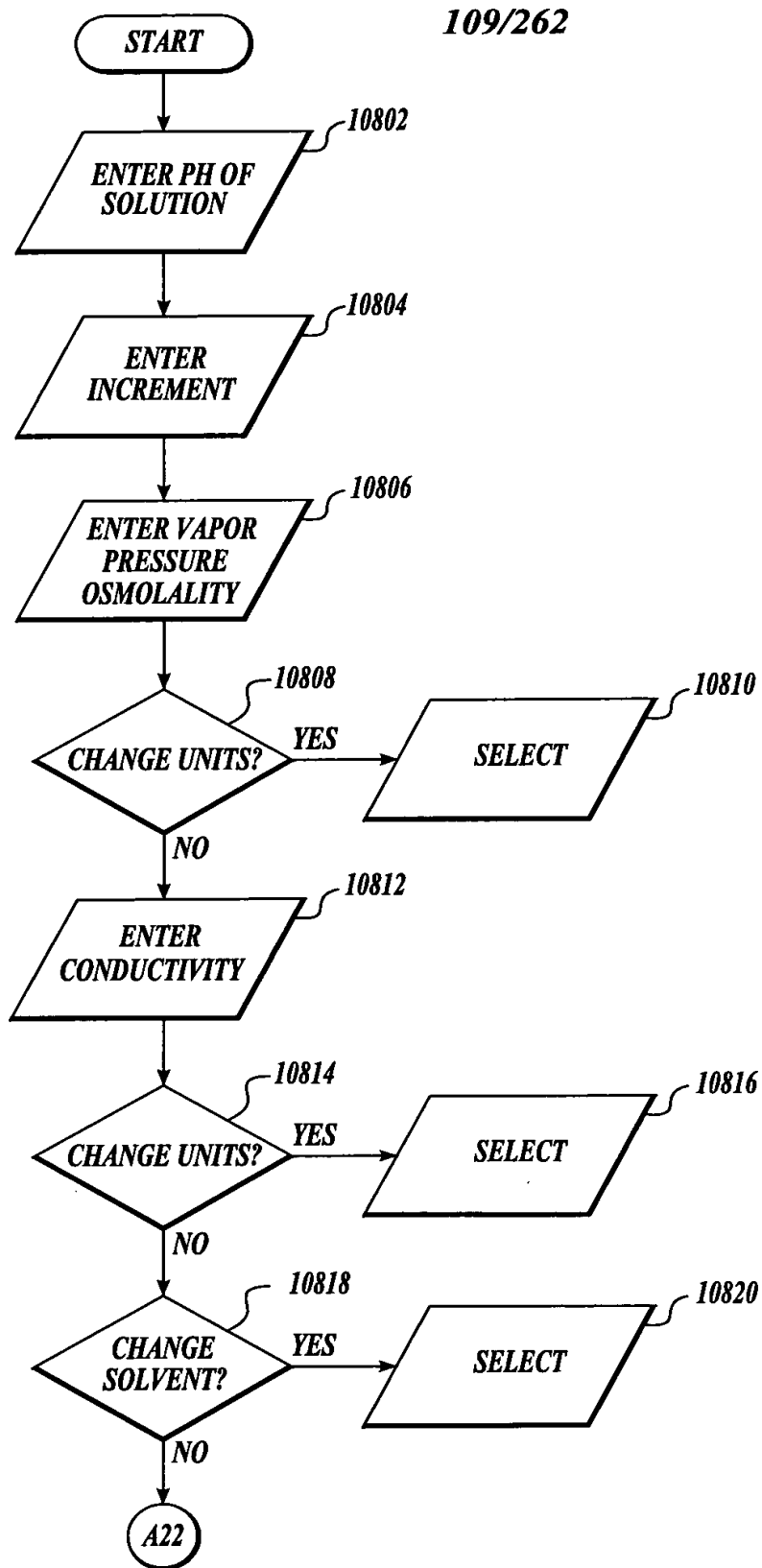


Fig. 108

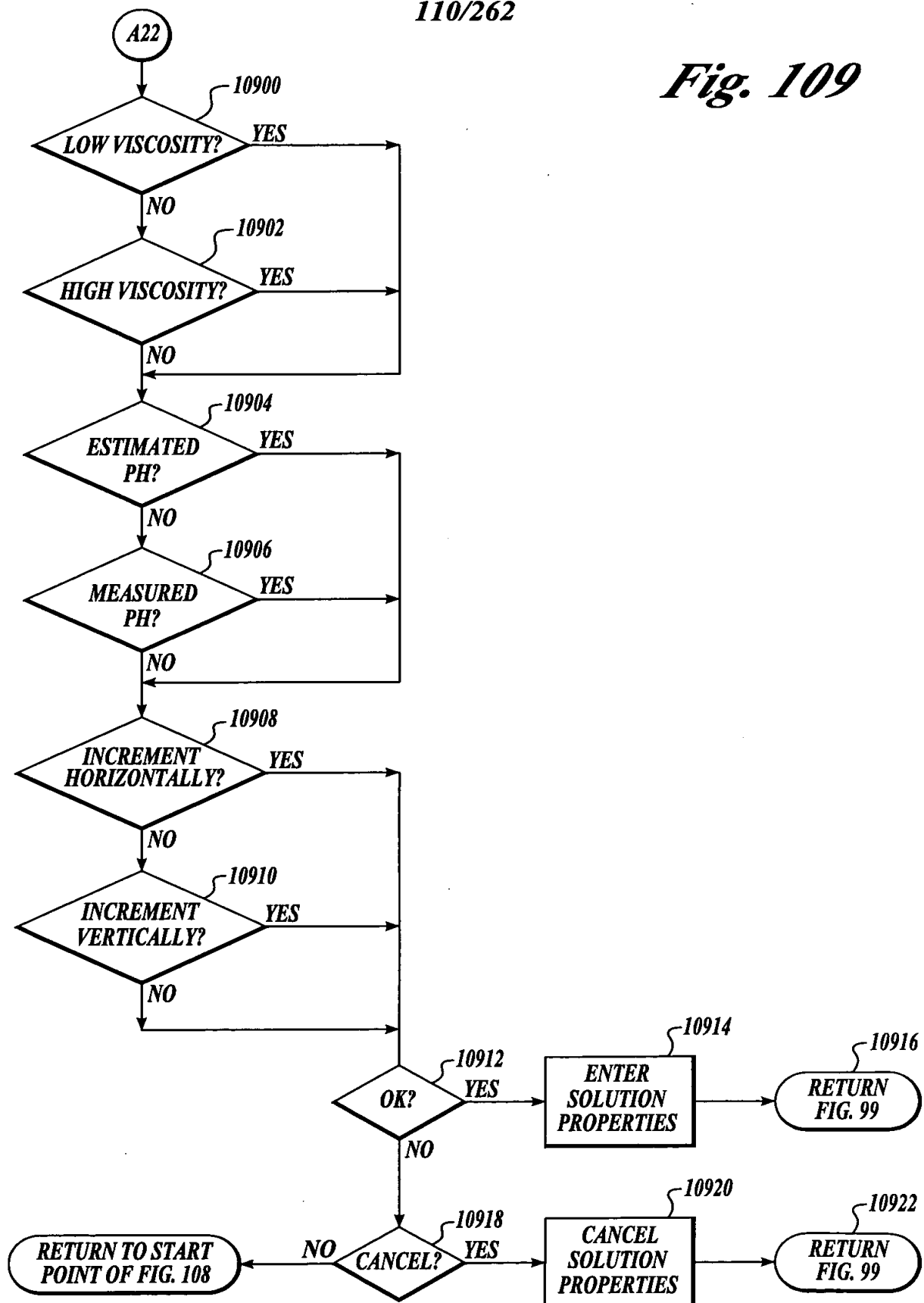
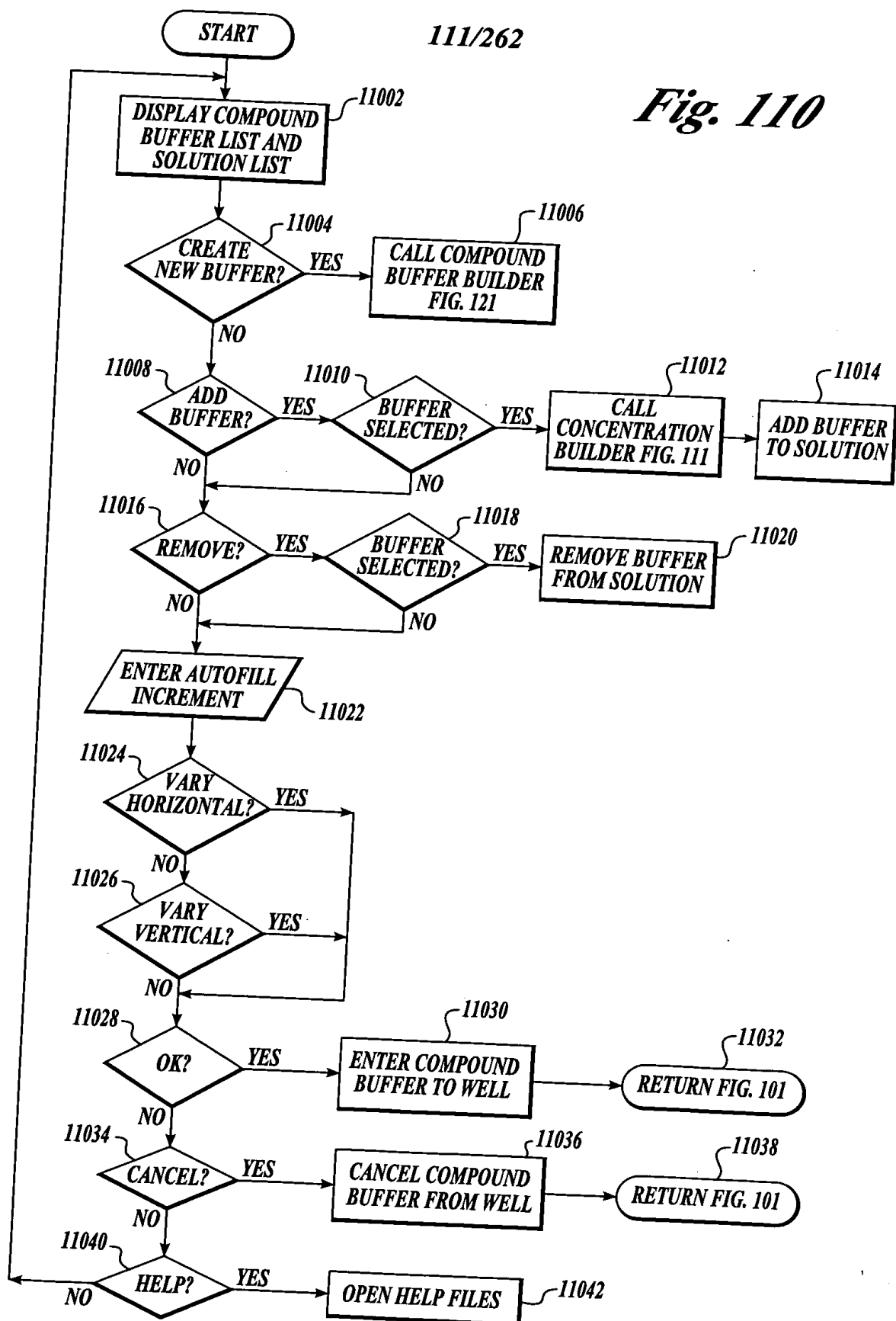
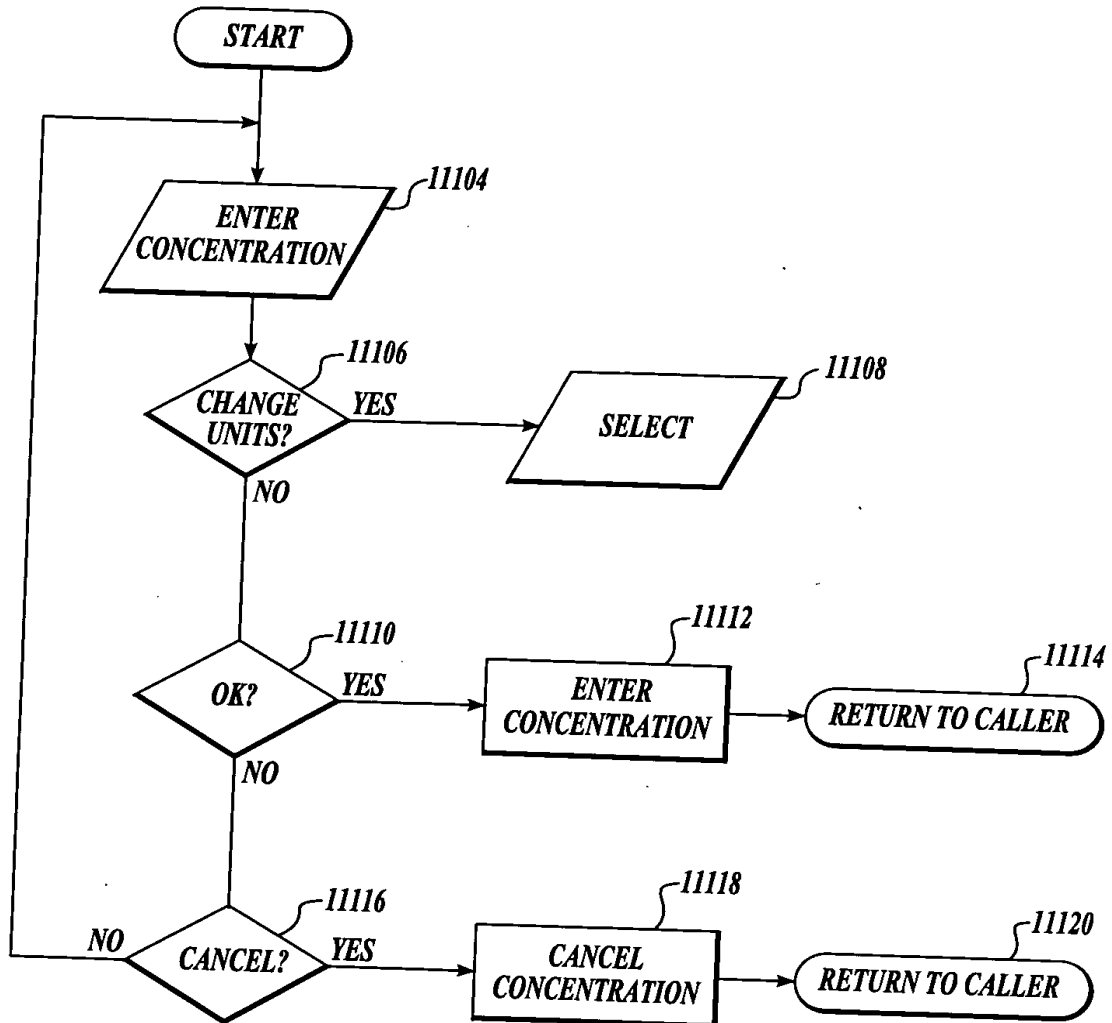
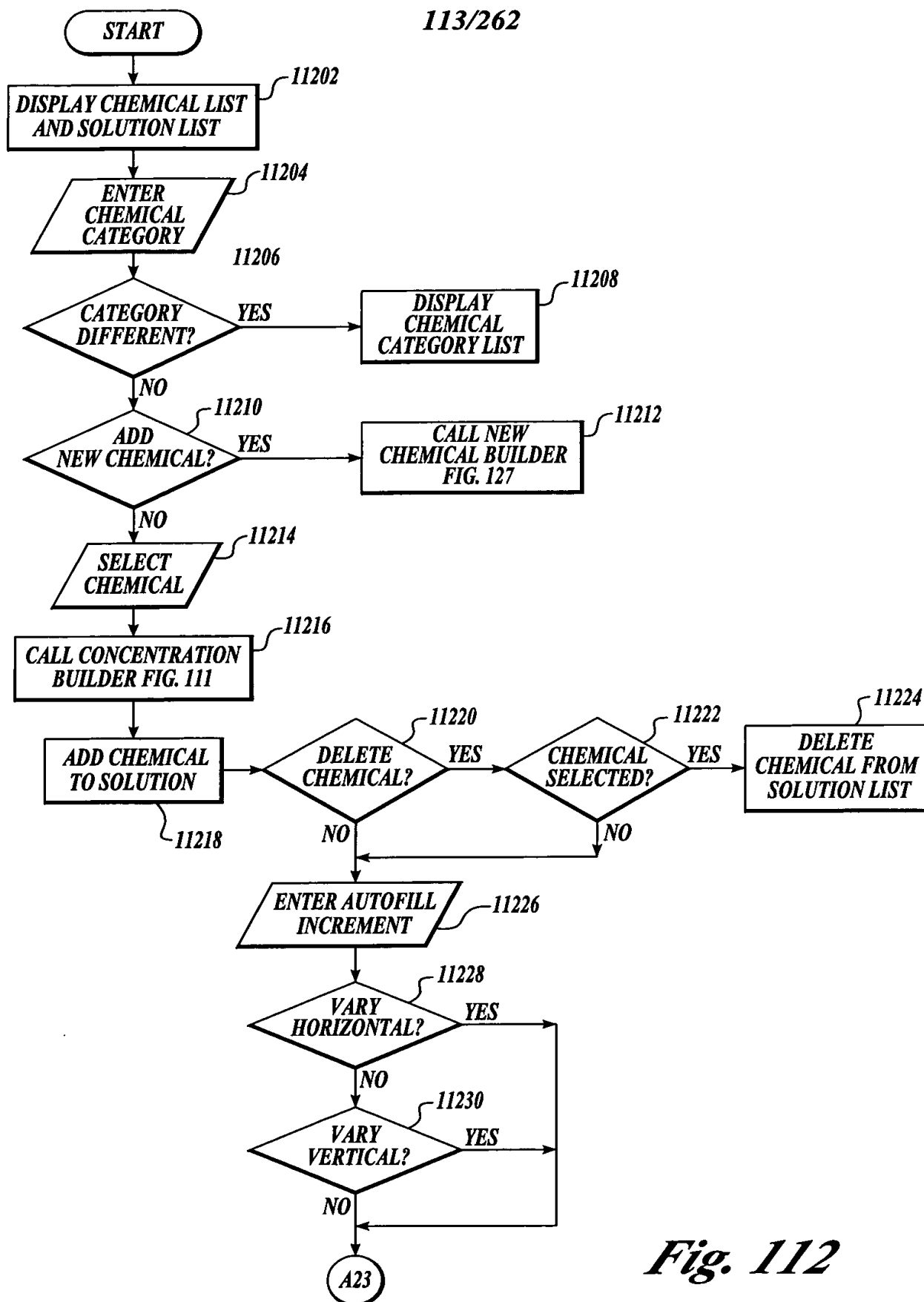
Fig. 109

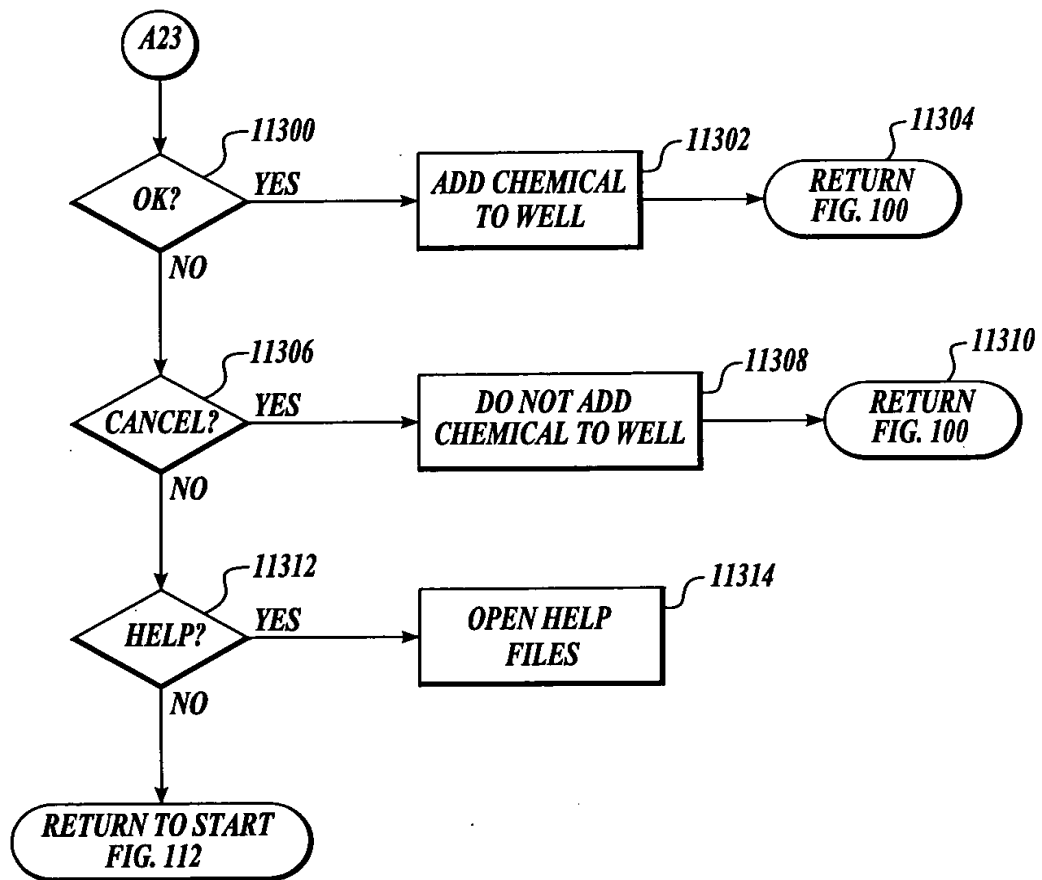
Fig. 110

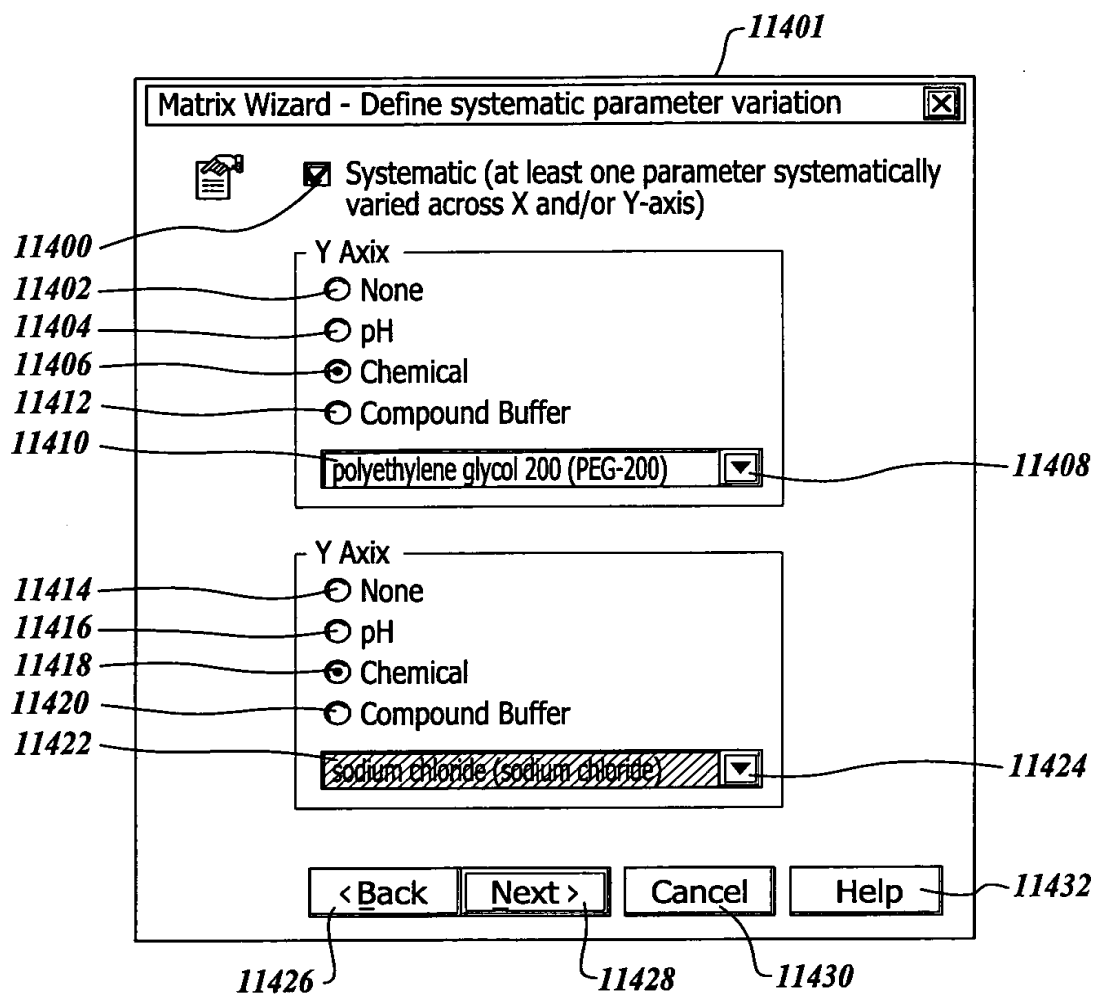


*Fig. 111*

113/262

*Fig. 112*

*Fig. 113*

*Fig. 114*

116/262

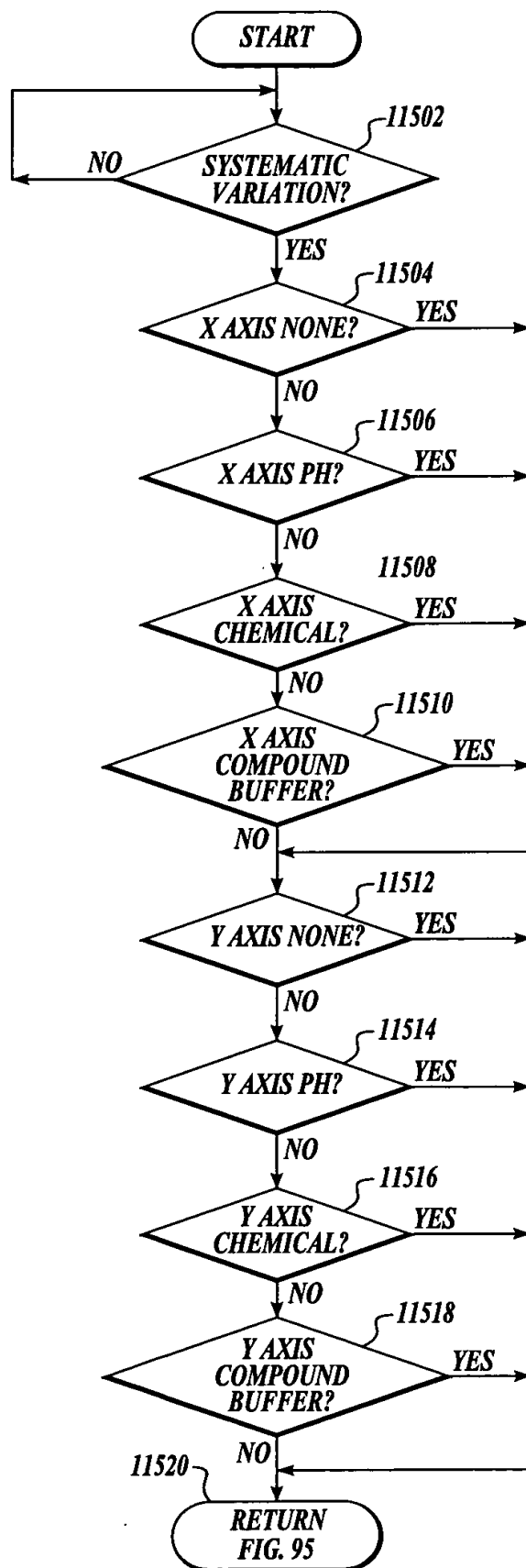
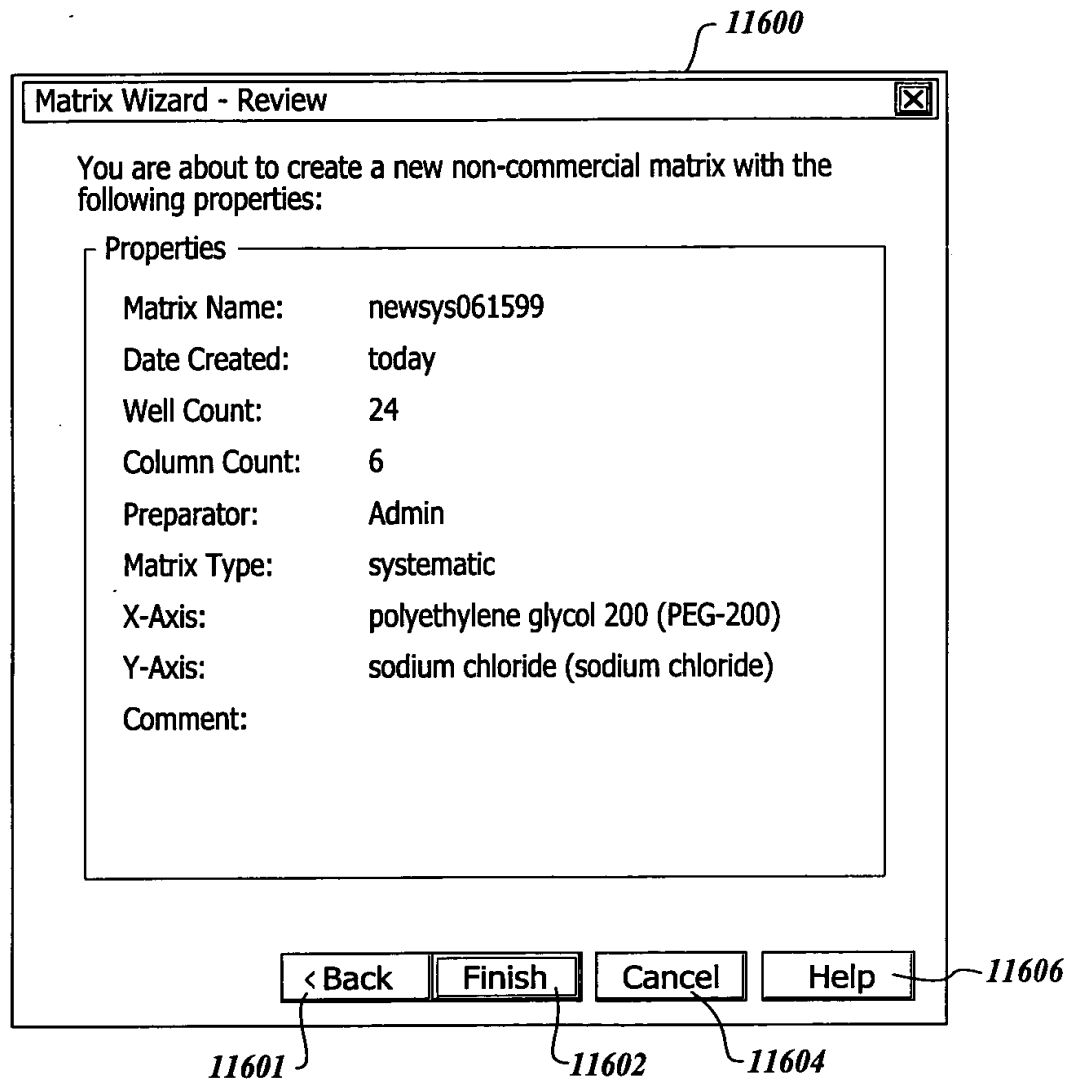
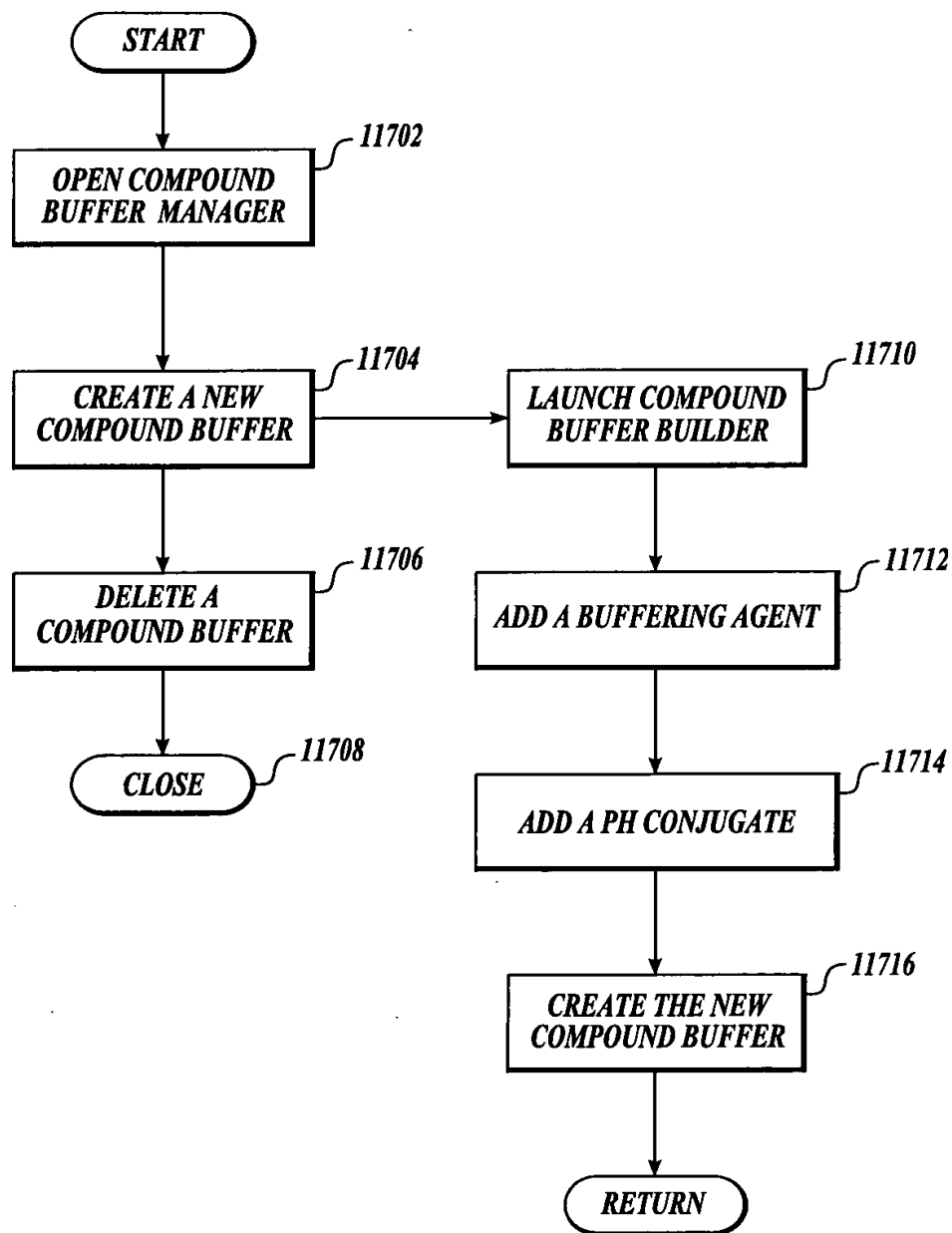


Fig. 115

*Fig. 116*

*Fig. 117*

11800

H⁺Compound Buffer Manager

Buffer PH	Buffering Agent (Full Name)	Buf Agent (abbr)	Buf Agent (Mntr)
H ⁺ 4.20	sodium phosphate dibasic	Na2 H phosphate	Sigma Chemical
H ⁺ 4.50	acetic acid	acetic acid	Sigma Chemical
H ⁺ 4.60	sodium acetate trihydrate	NaAc	Hampton Rese
H ⁺ 5.50	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Rese
H ⁺ 5.50	sodium citrate dihydrate	Na3 citrate	Sigma Chemical
H ⁺ 5.60	sodium citrate dihydrate	Na3 citrate	Hampton Rese
H ⁺ 5.60	2-morpholinoethanesulfonic acid	MES	Hampton Rese
H ⁺ 6.00	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Rese
H ⁺ 6.00	2-morpholinoethanesulfonic acid	MES	Hampton Rese
H ⁺ 6.00	(2-N-morpholino)ethanesulfonic acid	MES	Sigma Chemical
H ⁺ 6.20	sodium phosphate dibasic	Na2 H phosphate	Sigma Chemical
H ⁺ 6.50	sodium dimethylarsinic acid	Na cacodylate	Sigma Chemical
H ⁺ 6.50	n-(2-acetamido)iminodiacetic acid	ADA	Sigma Chemical
H ⁺ 6.50	sodium citrate dihydrate	Na3 citrate	Hampton Rese
H ⁺ 6.50	1,3-diaza-2,4-cyclopentadiene	imidazole	Hampton Rese
H ⁺ 6.50	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Rese
H ⁺ 6.50	2-morpholinoethanesulfonic acid	MES	Hampton Rese

New...

Delete

Help...

Close

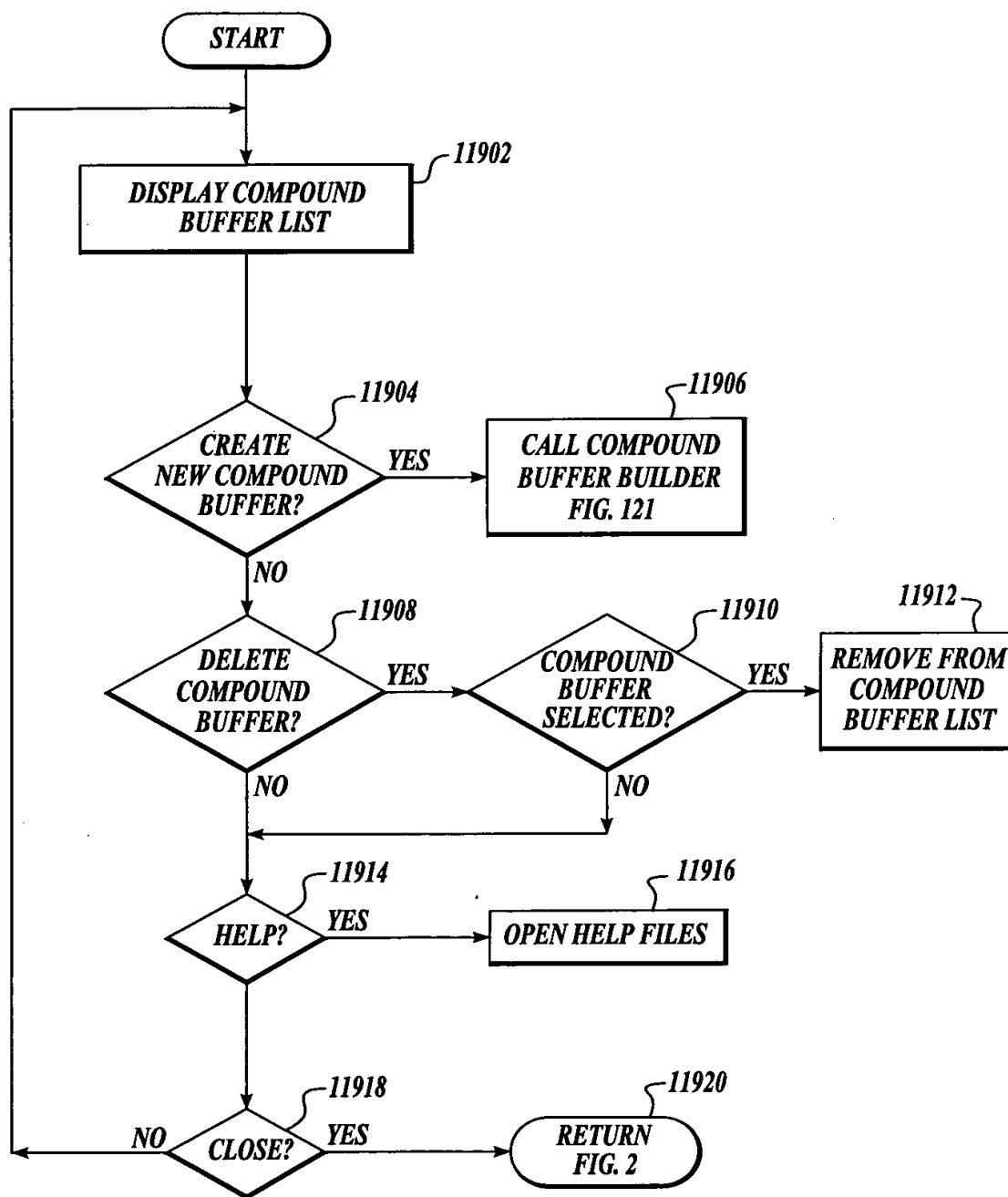
11808

11802

11804

11806

Fig. 118

*Fig. 119*

Compound Buffer Builder

Buffer Agent List:

Chemical Name	Abbreviation
acetic acid	acetic acid
cetyl trimethylammonium bromide	CTAB
citric acid monohydrate	citric acid
di-sodium hydrogen phosphate, dibasic	Na ₂ H phosphate

pH Conjugate (Counter Ion) List:

Chemical Name	Abbreviation
potassium dihydrogen phosphate, mon...	K H ₂ phosphate
sodium acetate	NaAc
sodium acetate trihydrate	NaAc
sodium cacodylic acid trihydrate	Na cacodylate

Compound Buffer Buffering Agent

Name: acetic acid
 Abbr: acetic acid (C₂H₄O₂)
 Mass: 60.05 Da
 Mfctr: Sigma Chemical Co.

Counter Ion:

Name: sodium acetate
 Abbr: NaAc (NaC₂H₃O₂)
 Mass: 82.03 Da
 Mfctr: Sigma Chemical Co.

Buffer pH (1..14): 4.9

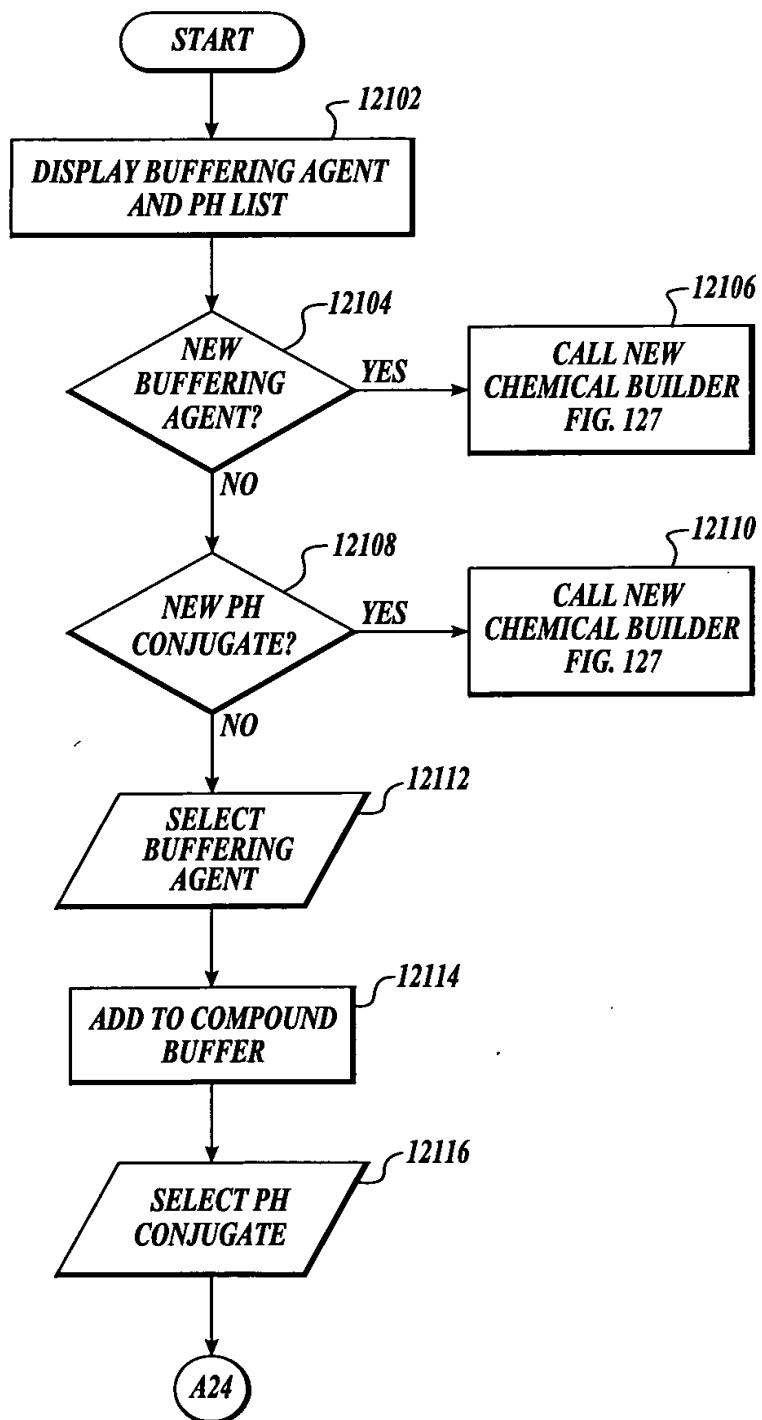
Comment: acetate buffer pH 4.9

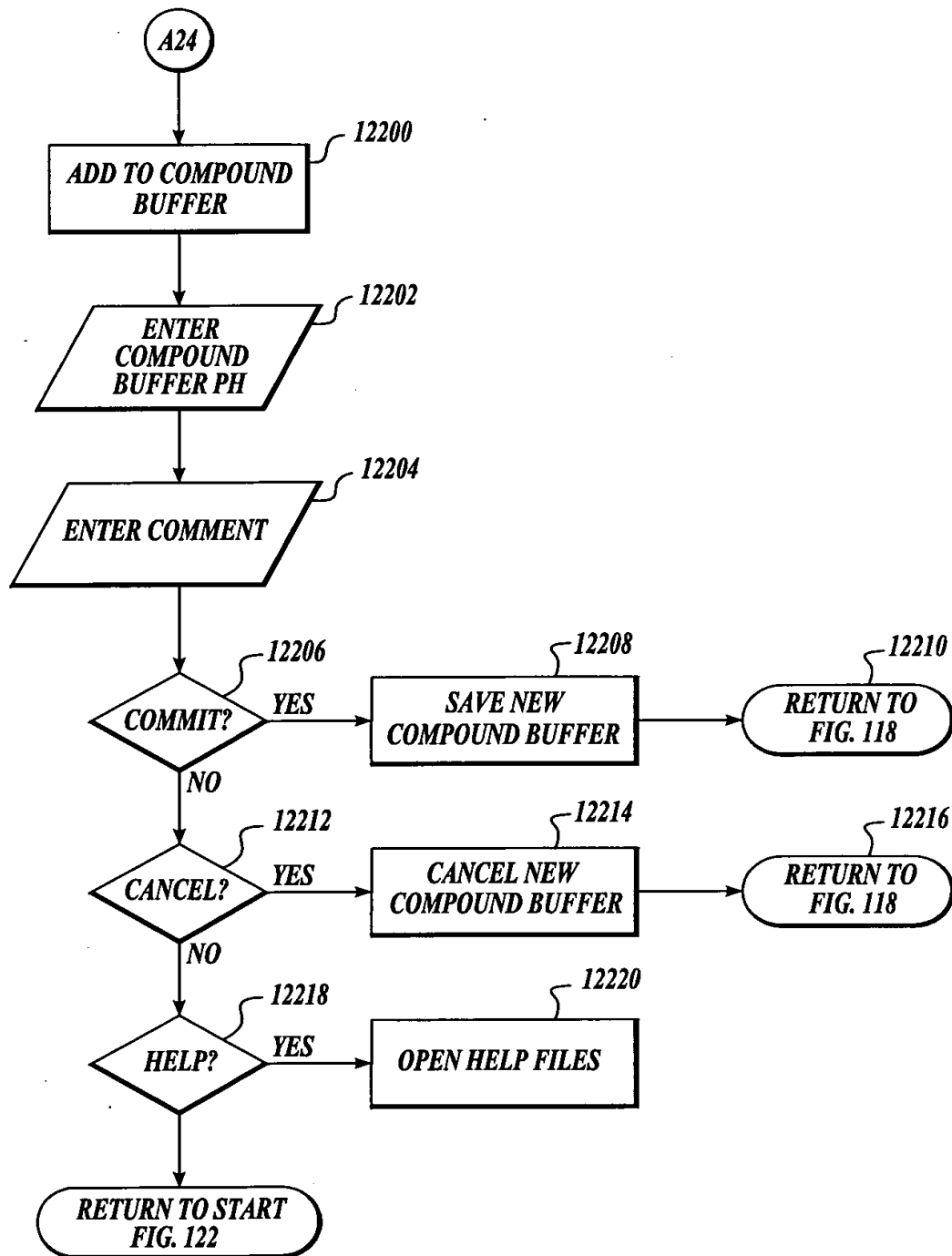
Compound Buffer

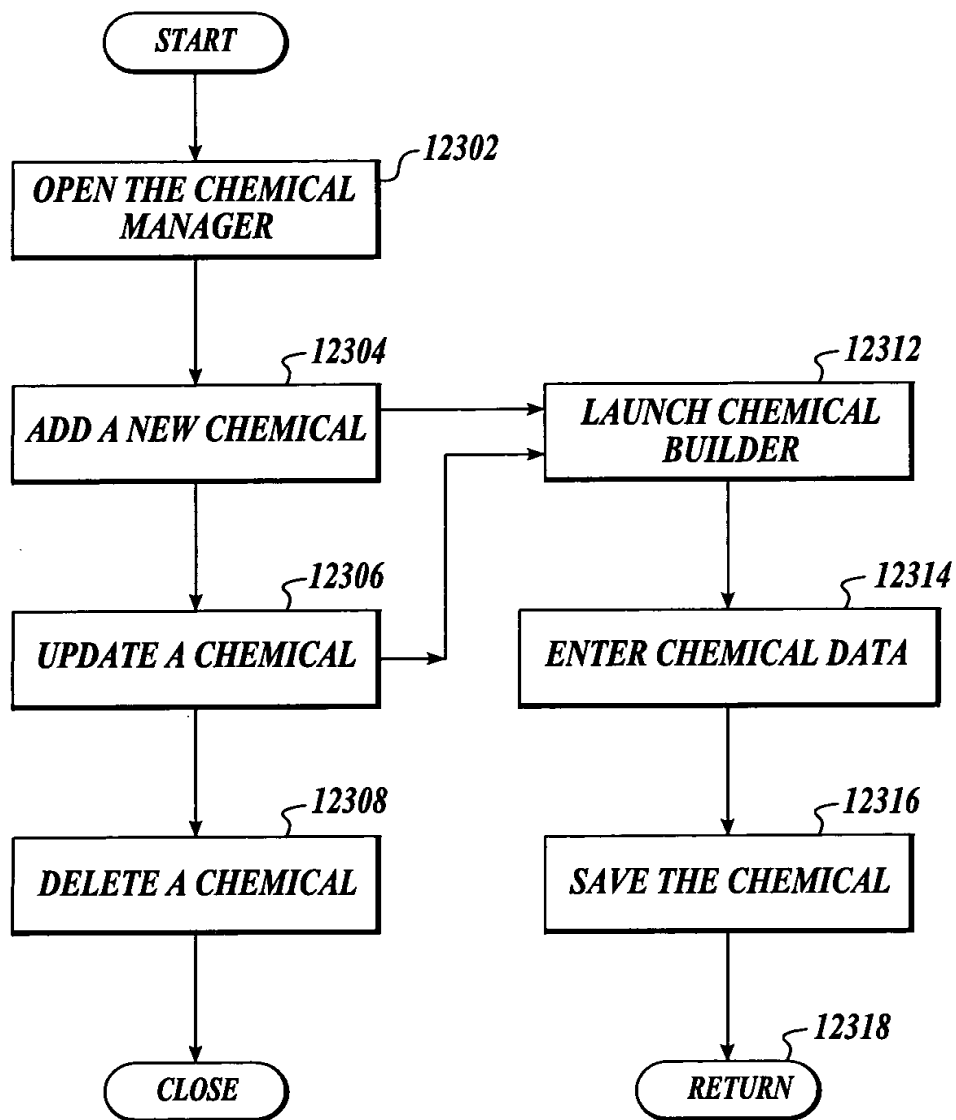
A Buffer is composed of exactly one Buffering Agent and exactly one pH Conjugate (Counter Ion).
 Double click on a Buffering Agent or pH Conjugate to copy the chemical to the right pane.

Commit Cancel Help...

Fig. 120

*Fig. 121*

*Fig. 122*

**Fig. 123**

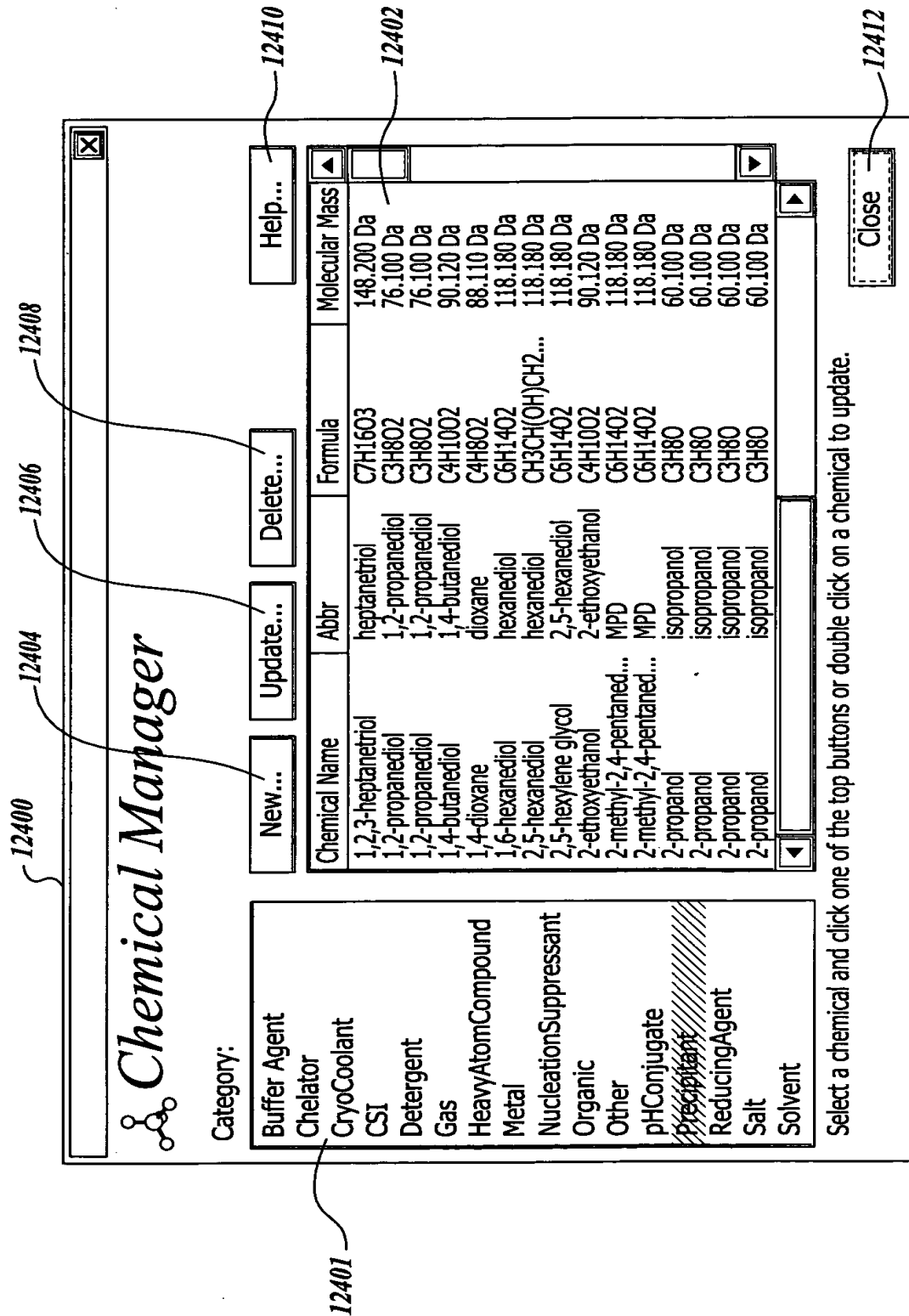


Fig. 124

12501

12510

New Chemical

12501 Name: ammonium sulfate

12502 Abbr: (NH₄)₂SO₄

Formula: (NH₄)₂SO₄

12504 Mass: 132.1 Da

12506 Chemical Type: Precipitant

12514 Density [g/ml]:

Manufacturer: Sigma Chemical Co.

12516 Catalog: A4915

12522 CAS: 7783-20-2

12524

State

☐ Gas

☐ Liquid

☒ Solid

12526

12508

12512

12520

12518

STOP

Warning

Catalog and CAS cannot be updated, once they have been entered, since they are the primary key for the chemical entity.

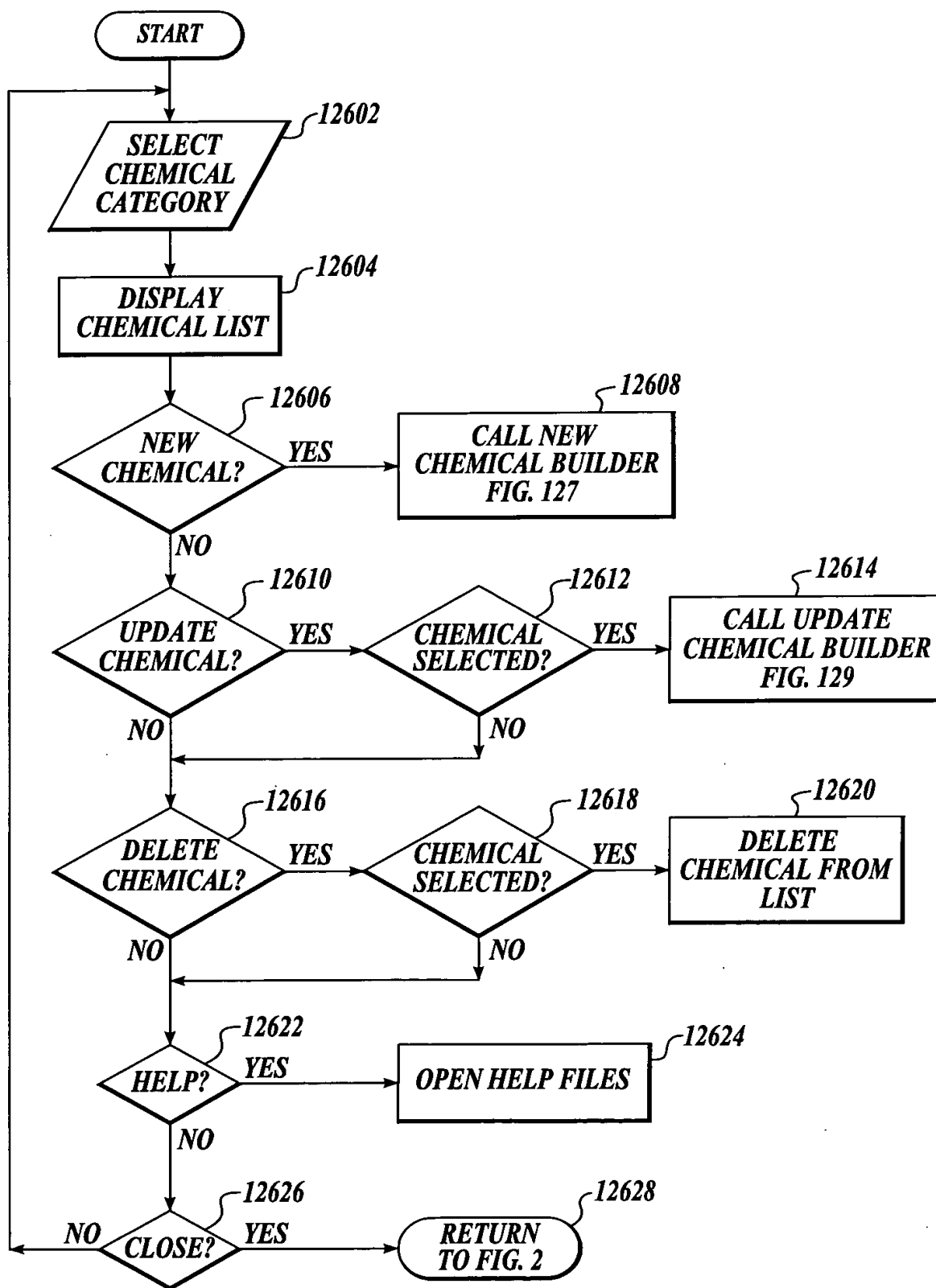
OK

Cancel

12528

12530

Fig. 125

*Fig. 126*

128/262

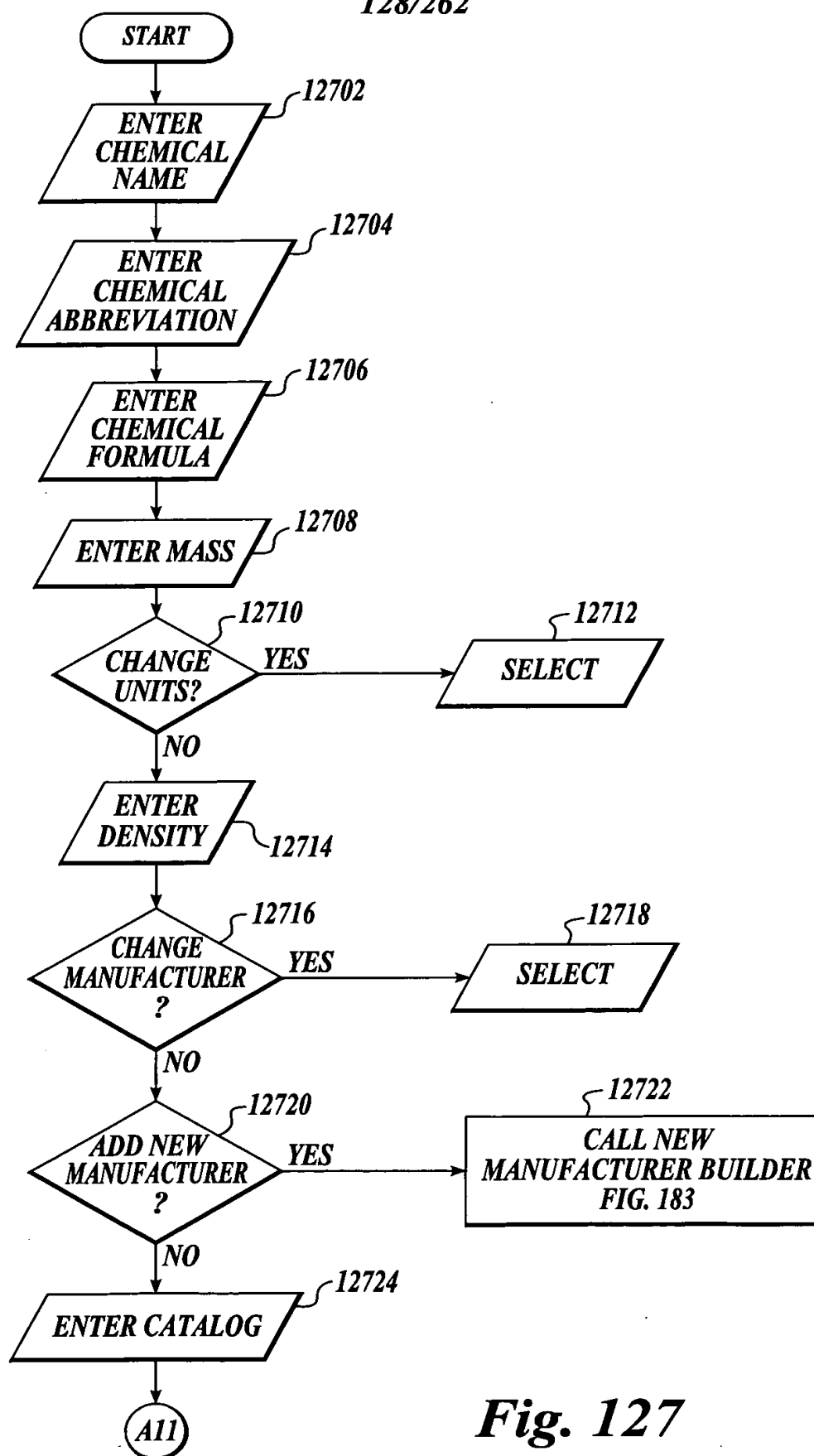
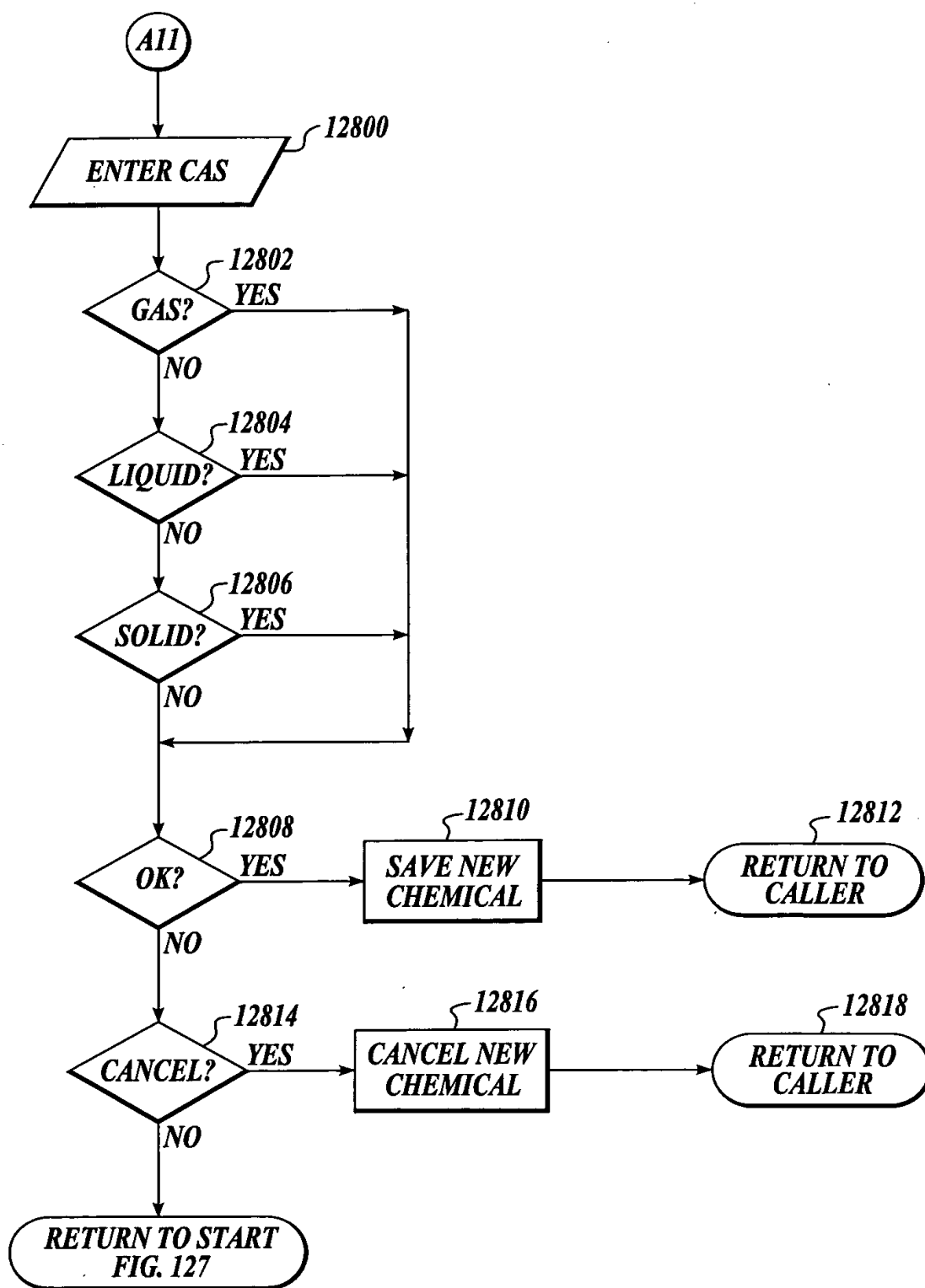
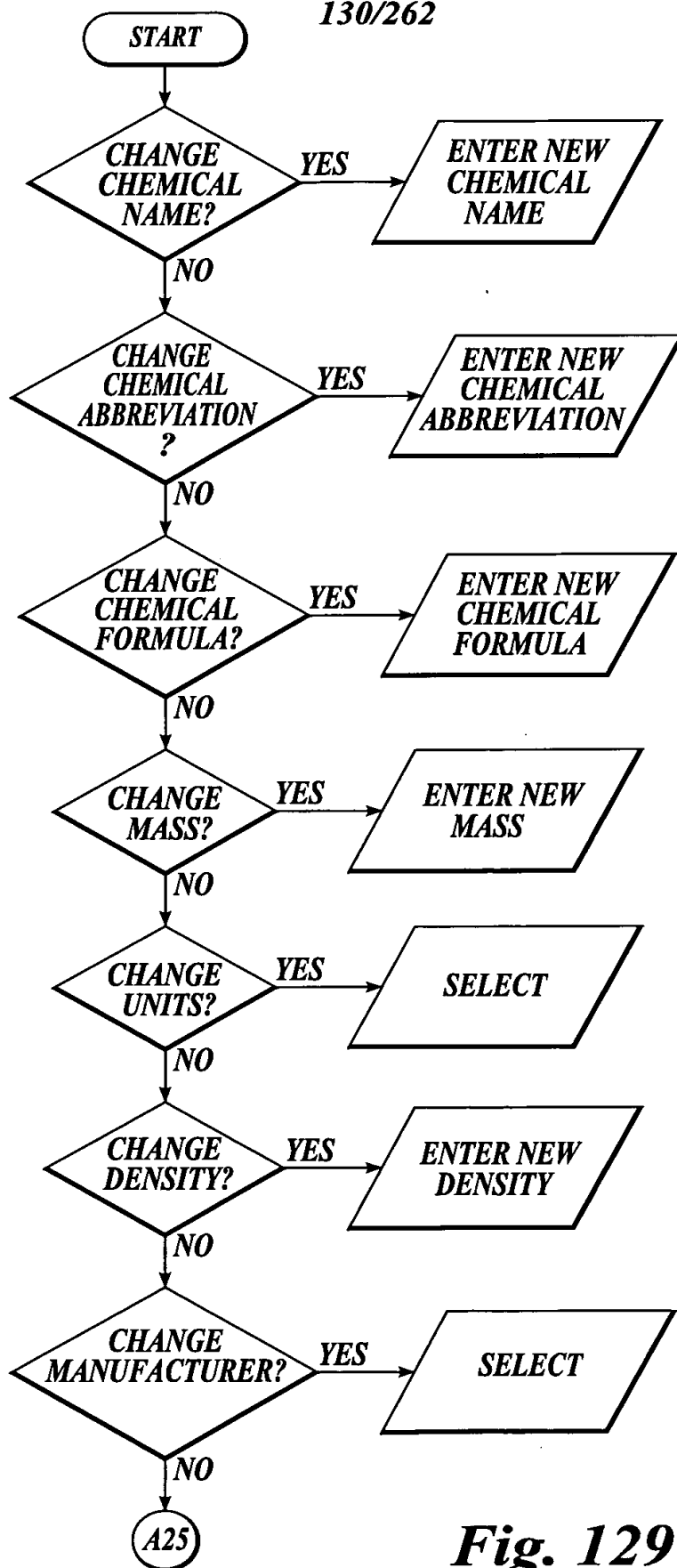
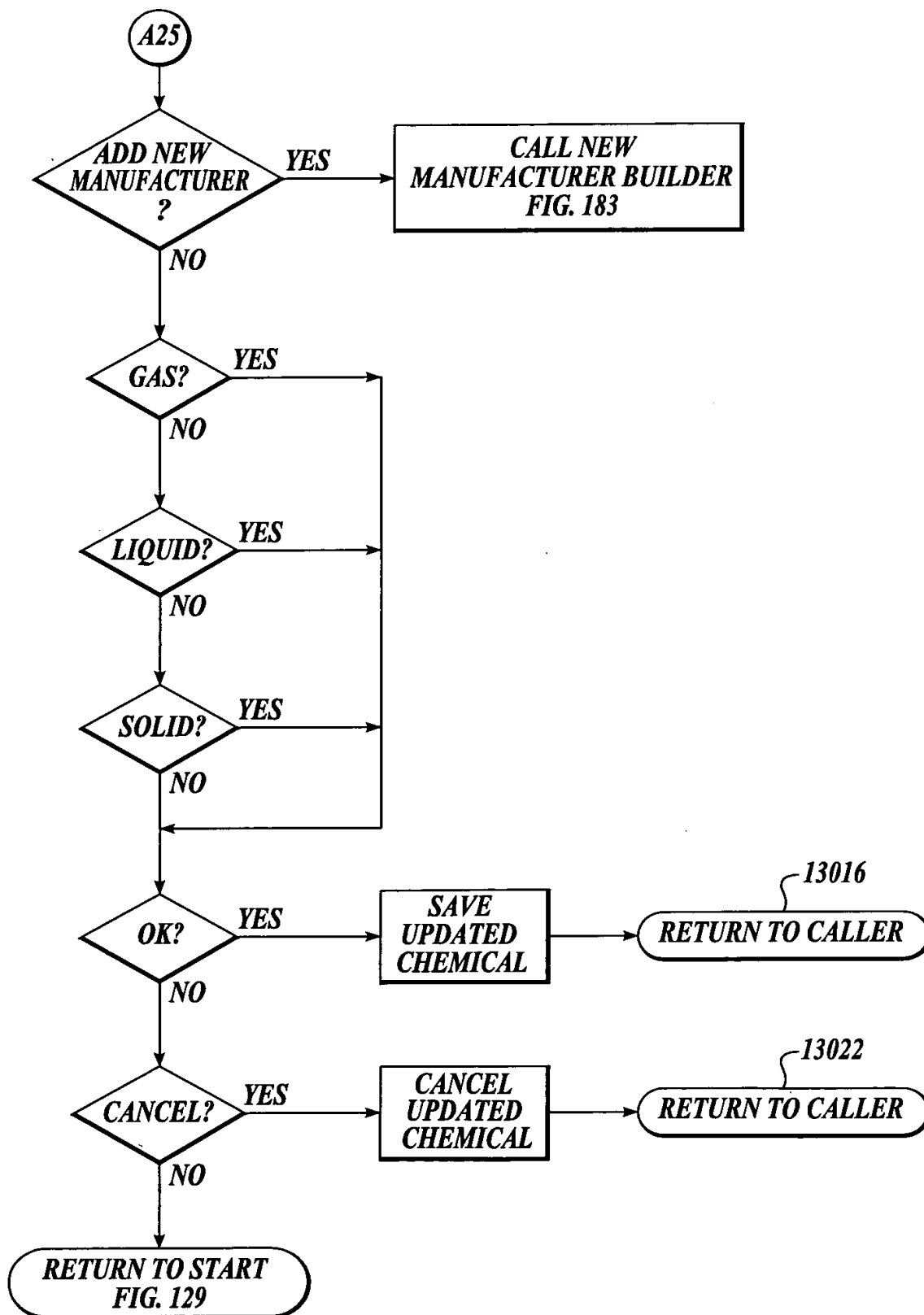


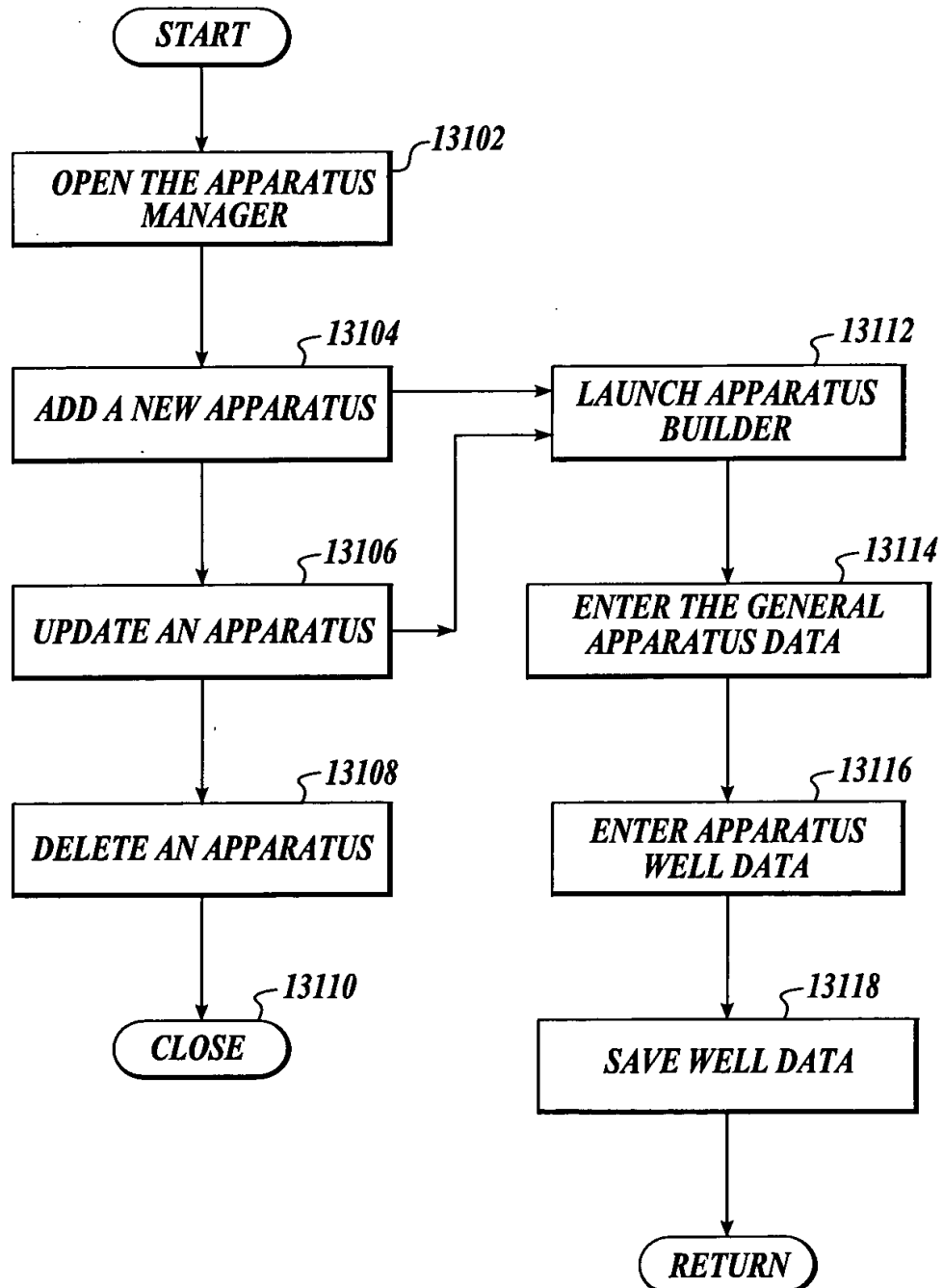
Fig. 127

*Fig. 128*

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**Fig. 129**

**Fig. 130**

**Fig. 131**

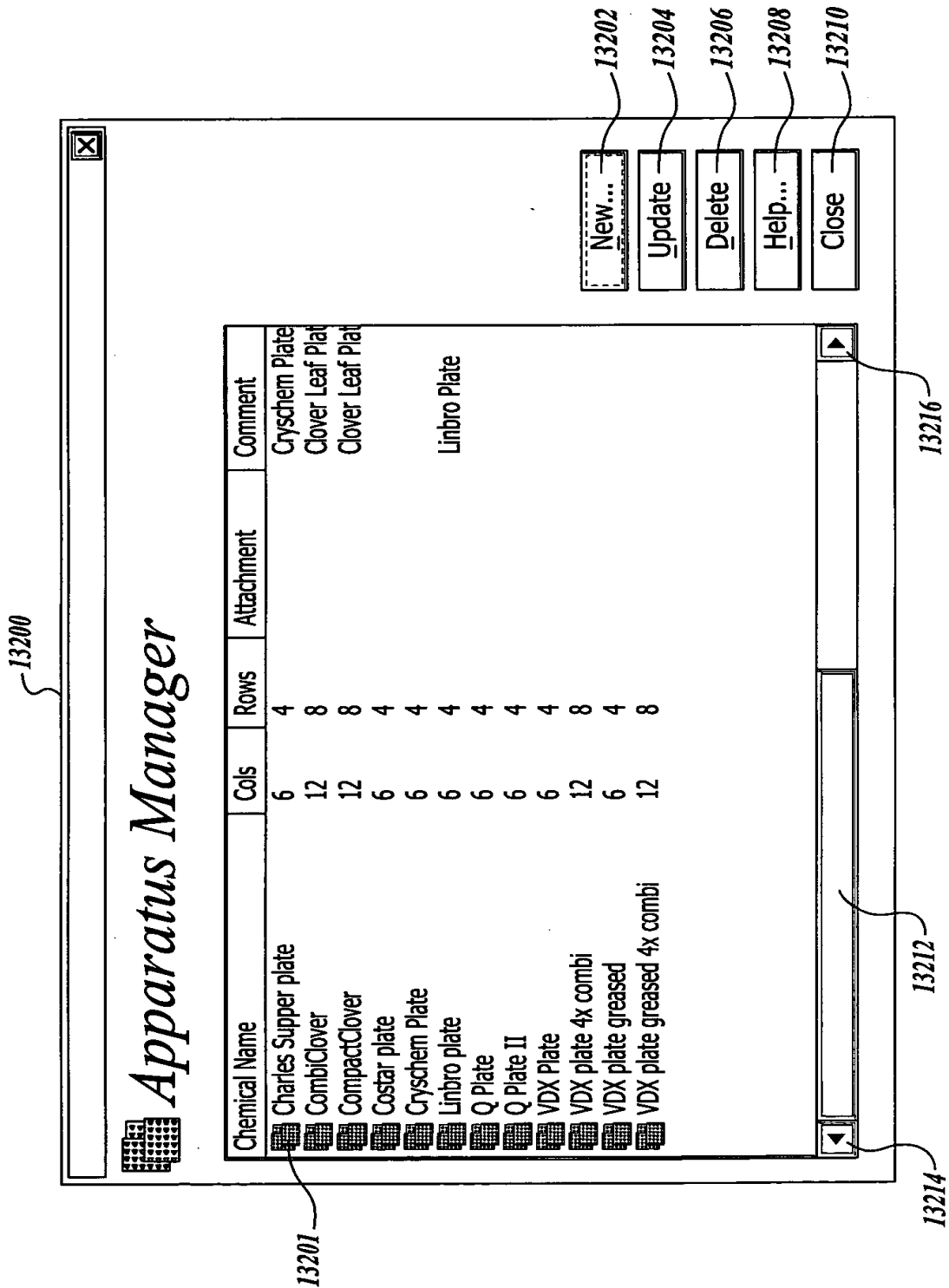
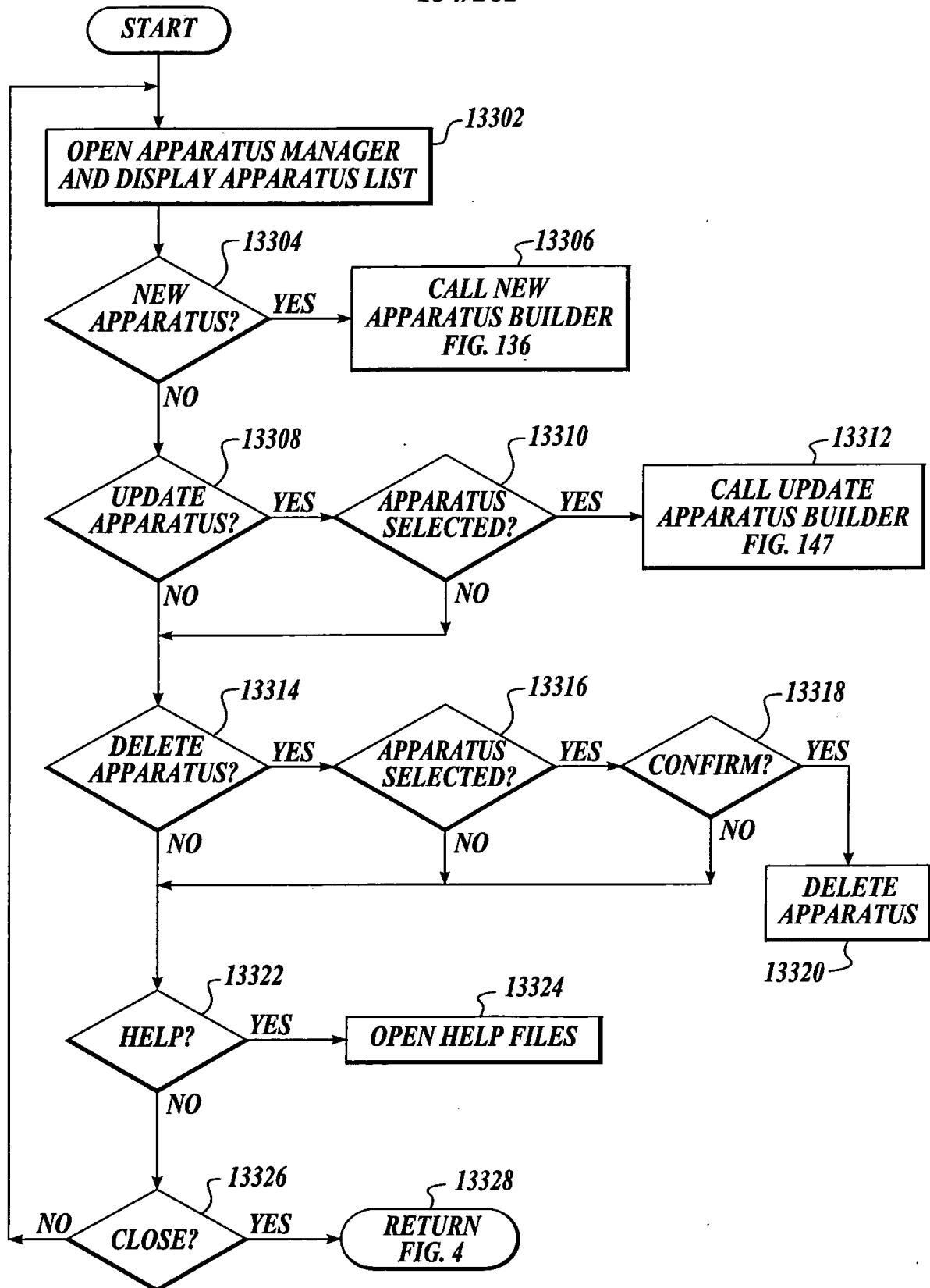


Fig. 132

*Fig. 133*

13401

13402

13400

New Apparatus

General apparatus data

Apparatus well data

13404

Name: CombiClover Jr.

13406

Manufacturer: Emerald BioStructures, Inc.

13410

Columns: 8 x Rows: 6

13414

Type: ☒ Crystallization ☐ Tube Rack

13418

Base dim (x,y,z): 112 75 20

Comment: 48-well CombiClover Jr. plate with standard microtiter plate footprint

Help

For more detailed help, please click the help button.

OK Cancel Help...

13420 13422 13424

13408

13419

E:\crymon\Help\crystalmonitor\images\coml

Fig. 134

13500

New Apparatus

General apparatus data Apparatus well data

AutoFill... 13501

1	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	2	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	3	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	4	x y	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:
9	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	10	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	11	x y z	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	12	x y	Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:
17	x y z	Drop:	18	x y z	Drop:	19	x y z	Drop:	20	x y	Drop:

OK 13502 Cancel 13504 Help... 13506

Fig. 135

137/262

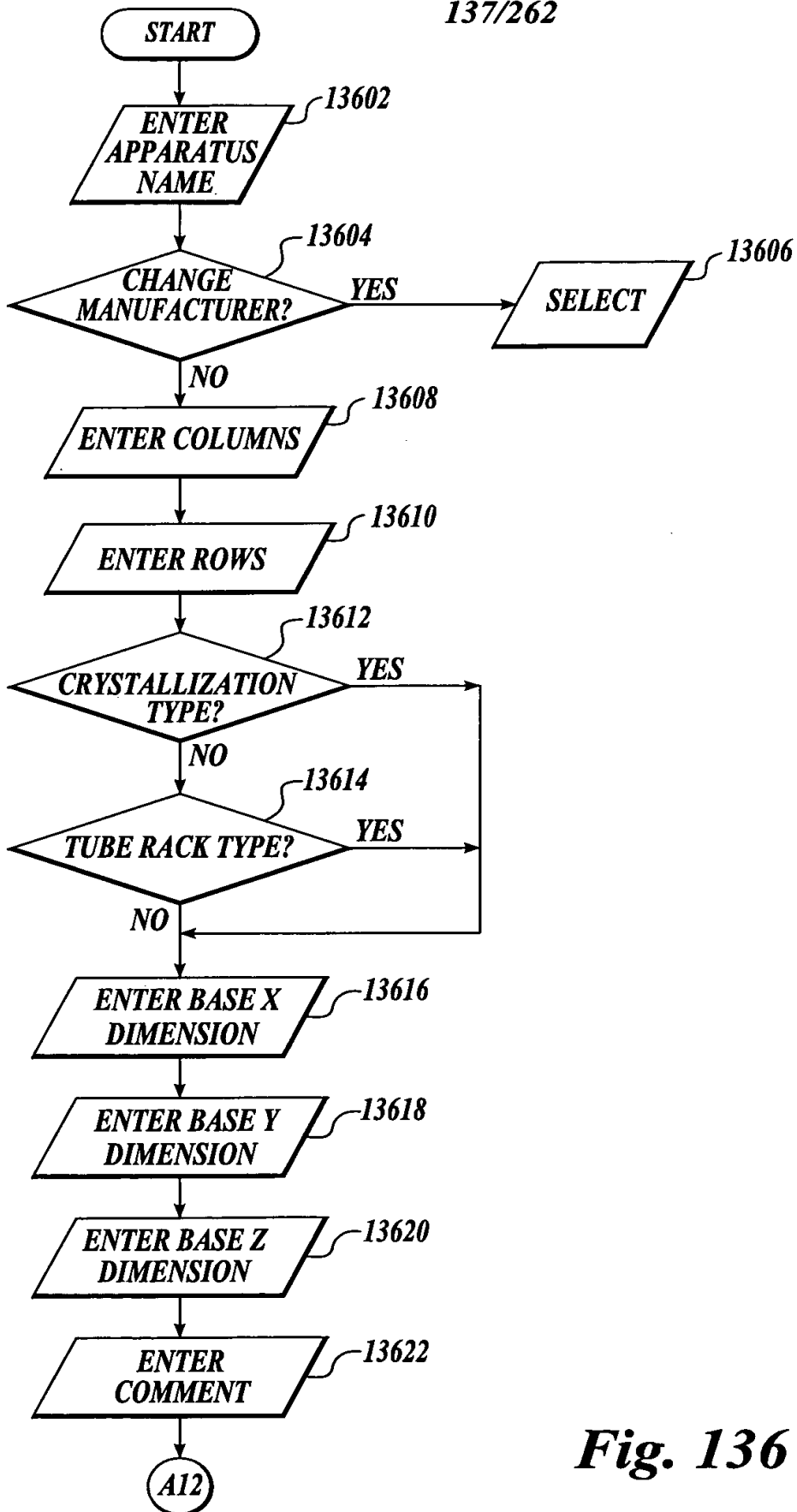
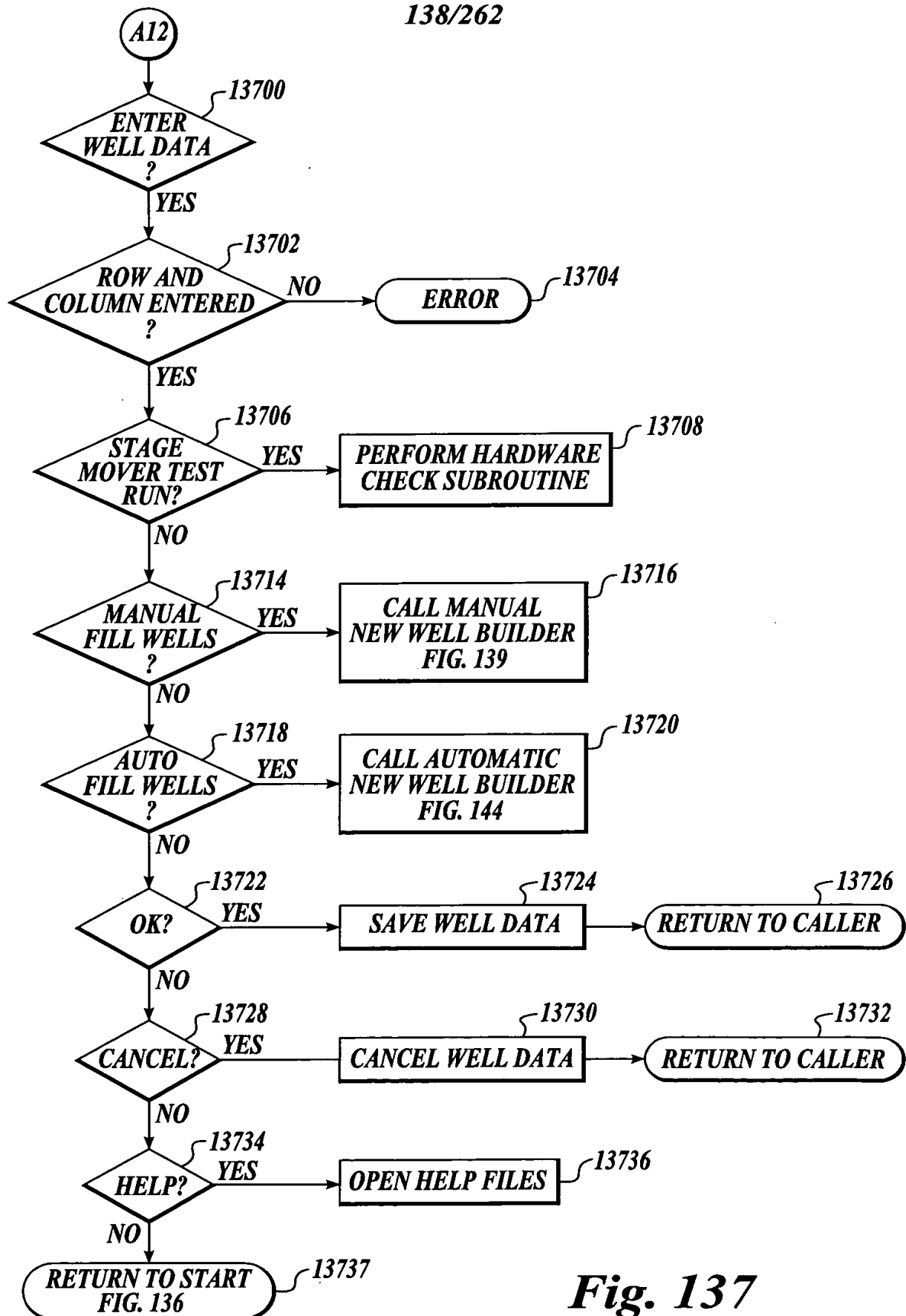


Fig. 136

*Fig. 137*

13800

Updating Well #1

Well coordinates in millimeter (mm)

	X	Y	Z	Diameter
Drop chamber:	10	5	5	5
Res. Chamber	15	10	20	10

Volume

Max Vol Drop Chamber: 30 μ l

Max Vol Res. Chamber: 1000 μ l

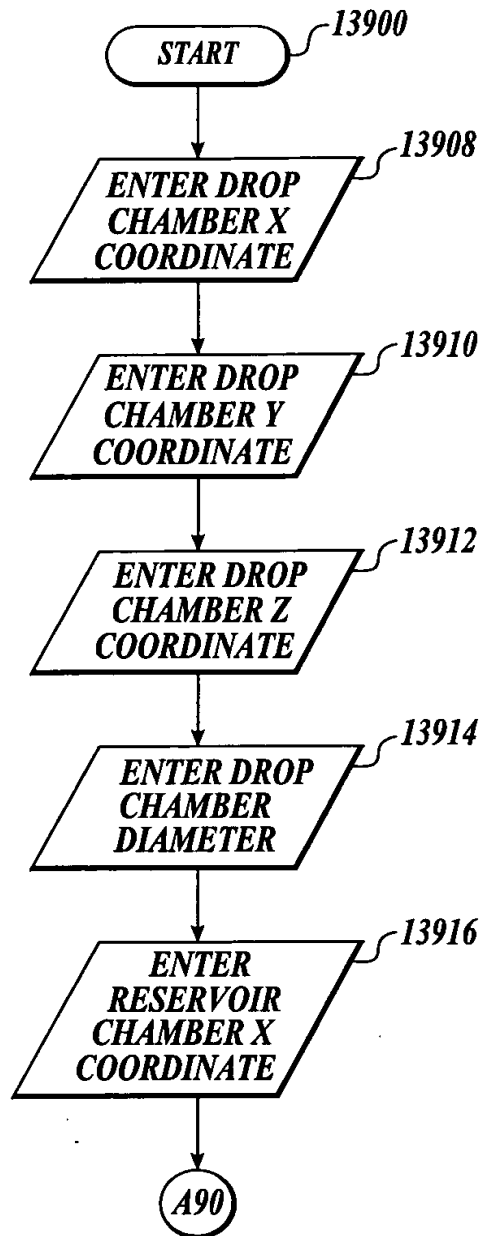
Help...

OK

Cancel

13804 — Drop chamber: 10 5 5 5 — 13801
13808 — Res. Chamber 15 10 20 10 — 13806
13809 — 13810
13812
13814
13802
13820
13818
13816
13822 — Help... — 13824
13826 — Cancel

Fig. 138

**Fig. 139**

141/262

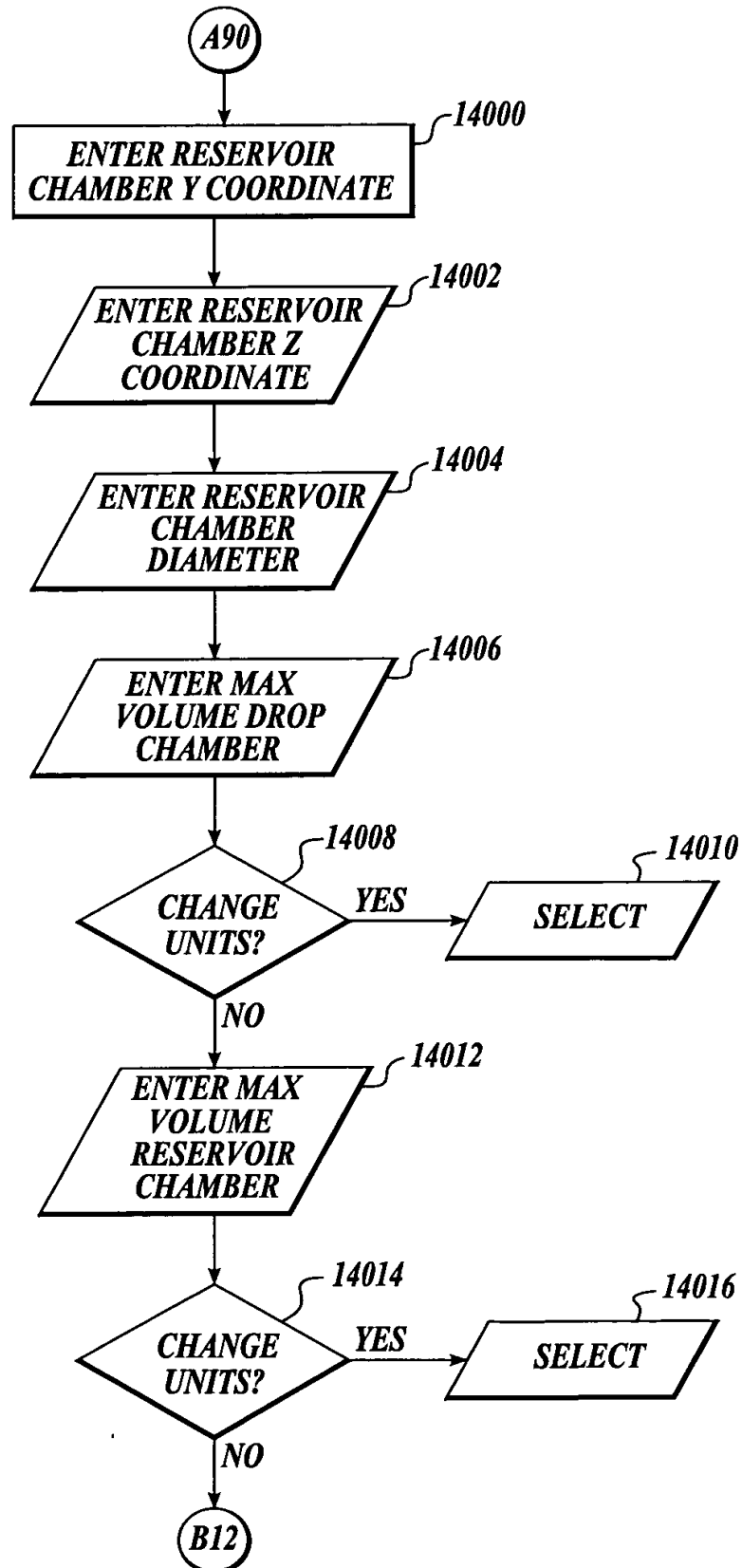
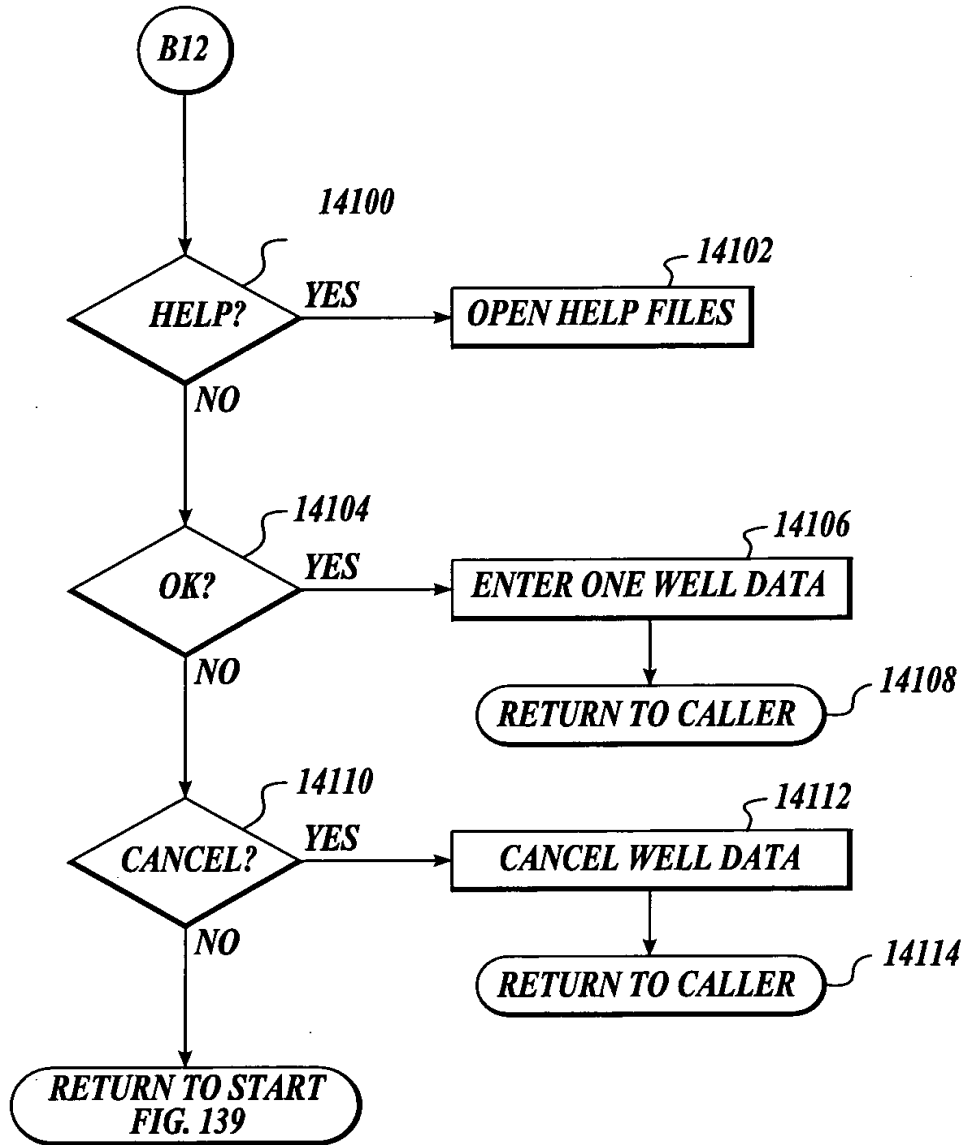


Fig. 140

**Fig. 141**

Autofill Apparatus Coordinates

Chamber coordinates in millimeters

	Drop	Reservoir
(1)	15	20
(2)	5	10
(3)	5	20
(4)	15	15
(5)	15	15
Diam.	5	10

Max Chamber Volume

Drop: 30 μ l

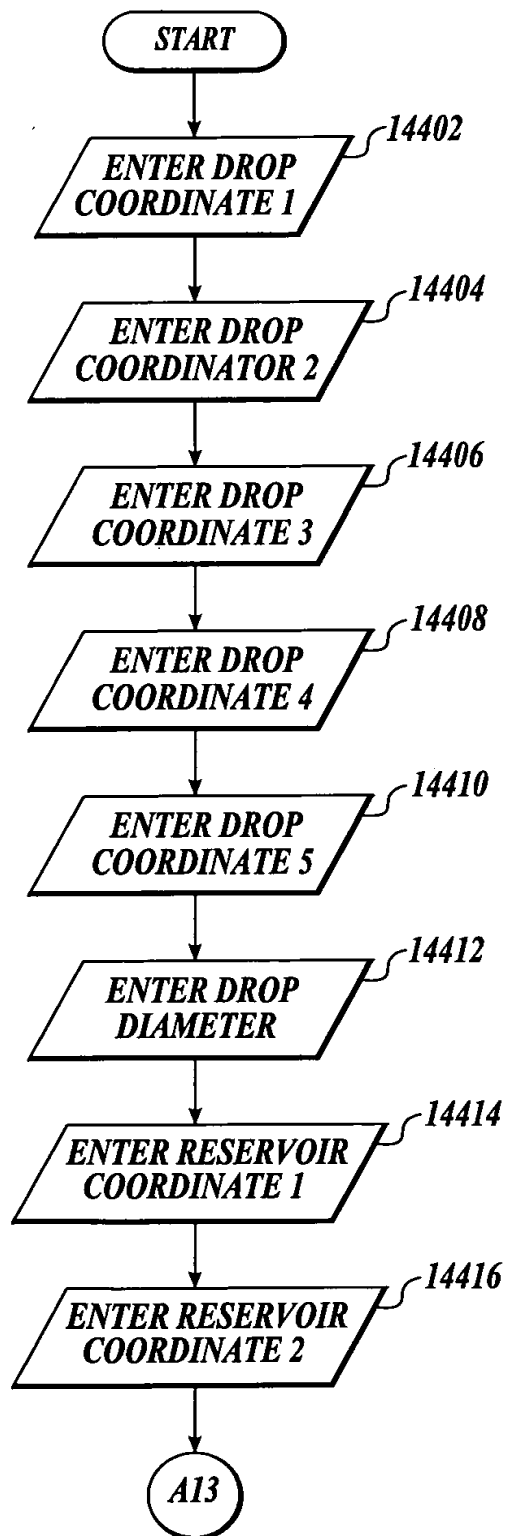
Reservoir: 1000 μ l

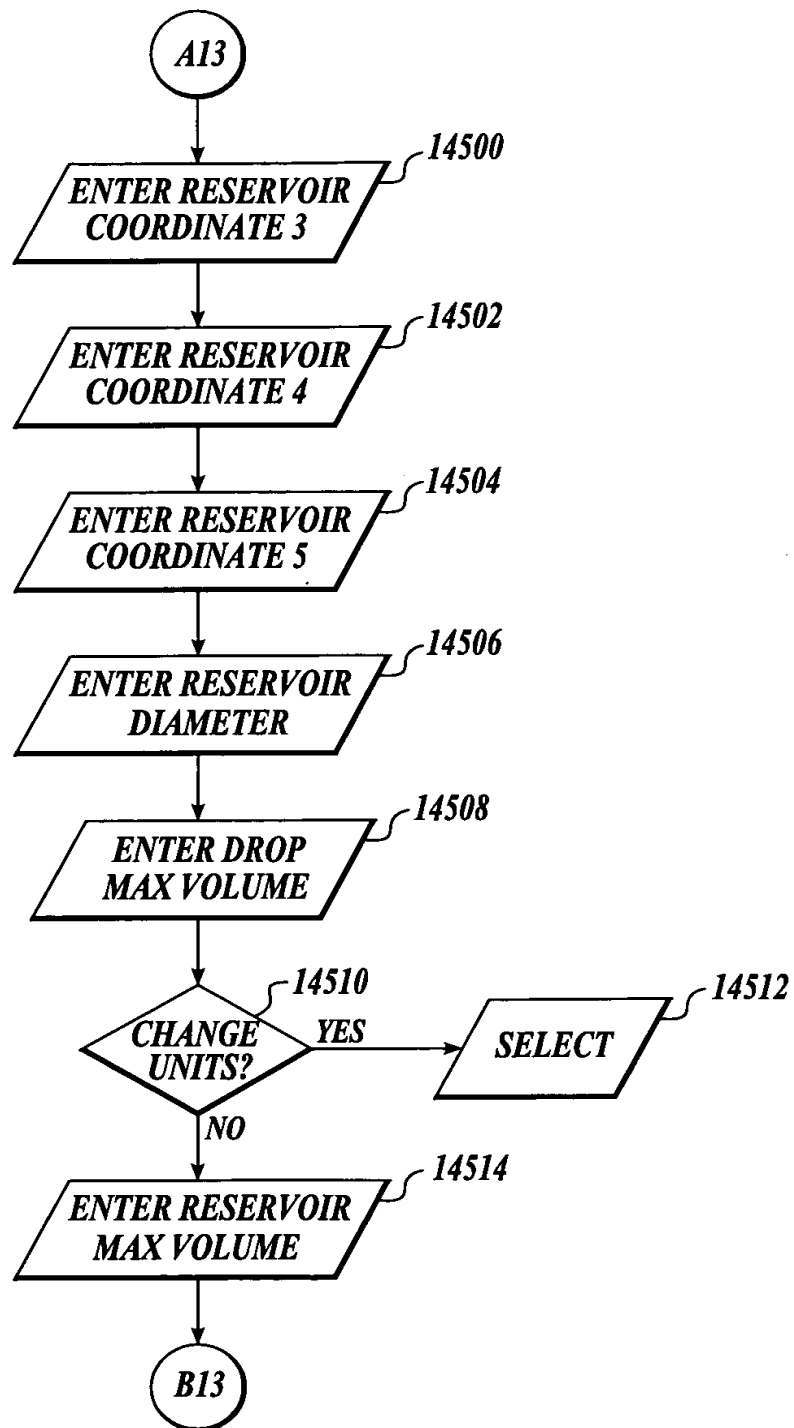
Hint
Autofill helps reducing to enter all the coordinates to fully describe a plate. It assumes that the plate has symmetric attributes, so that the above coordinates describe the plate uniquely.
You can overwrite coordinates afterwards by double clicking on a well.

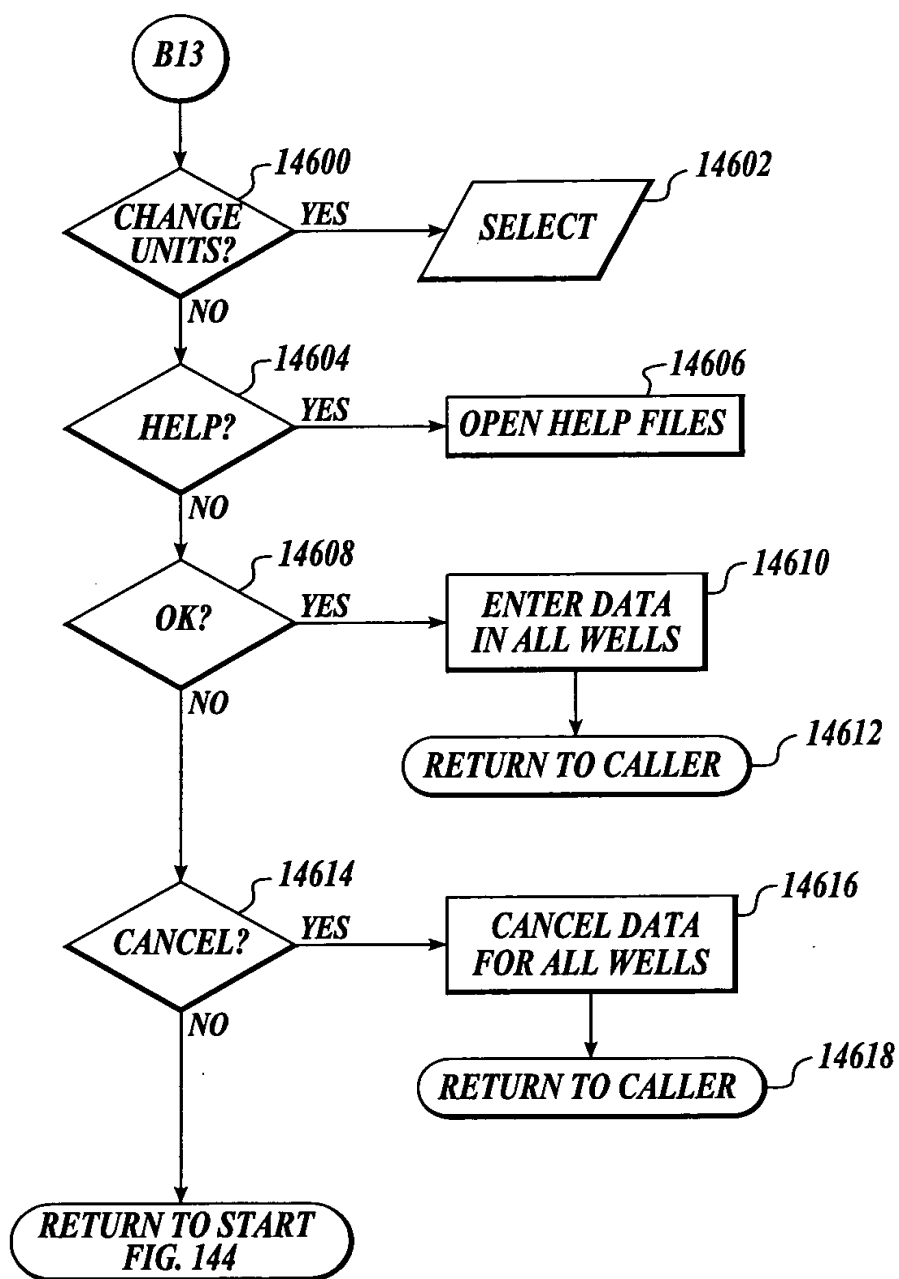
Help... OK Cancel

Fig. 142

Fig. 143

**Fig. 144**

**Fig. 145**

**Fig. 146**

148/262

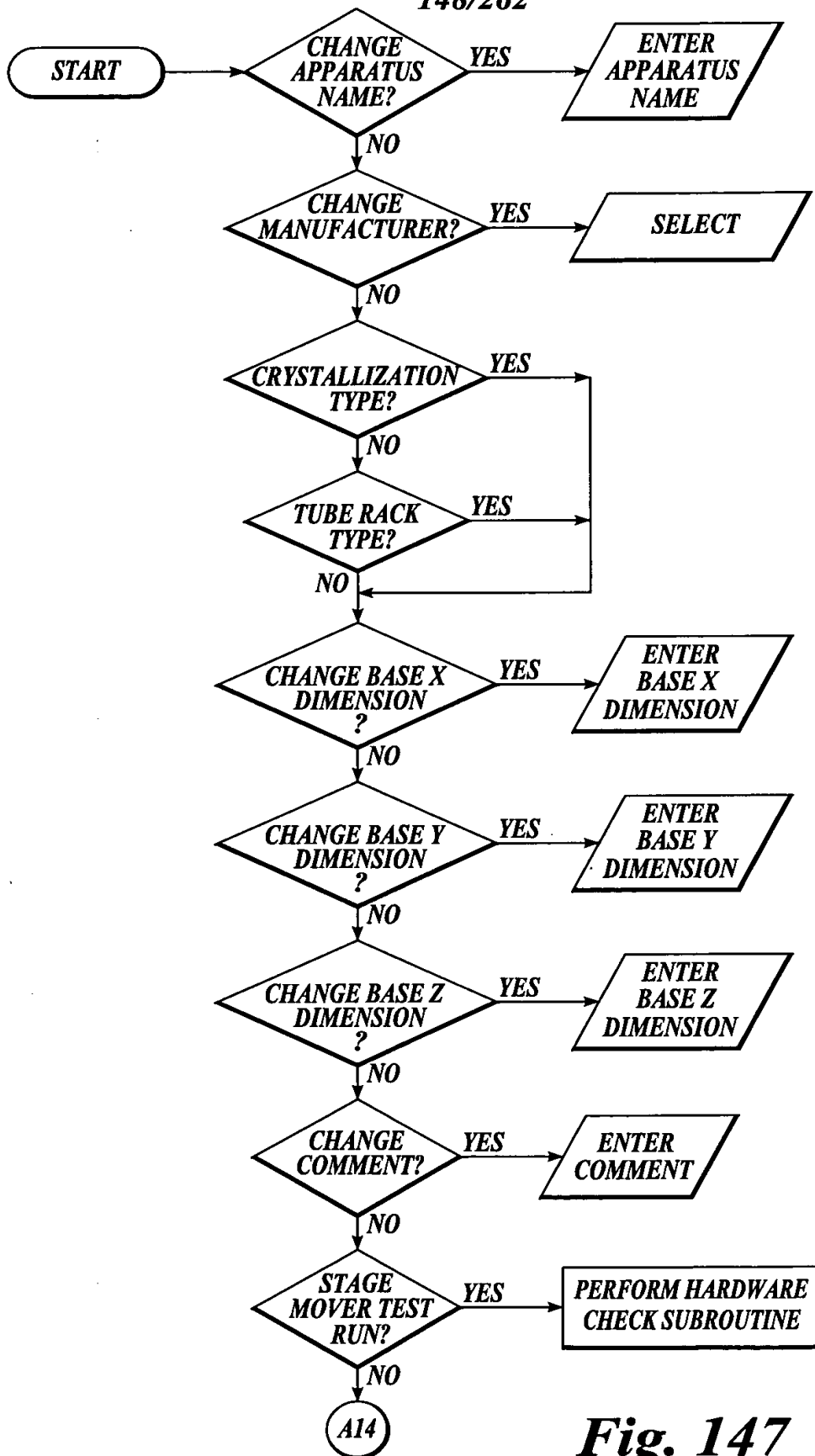
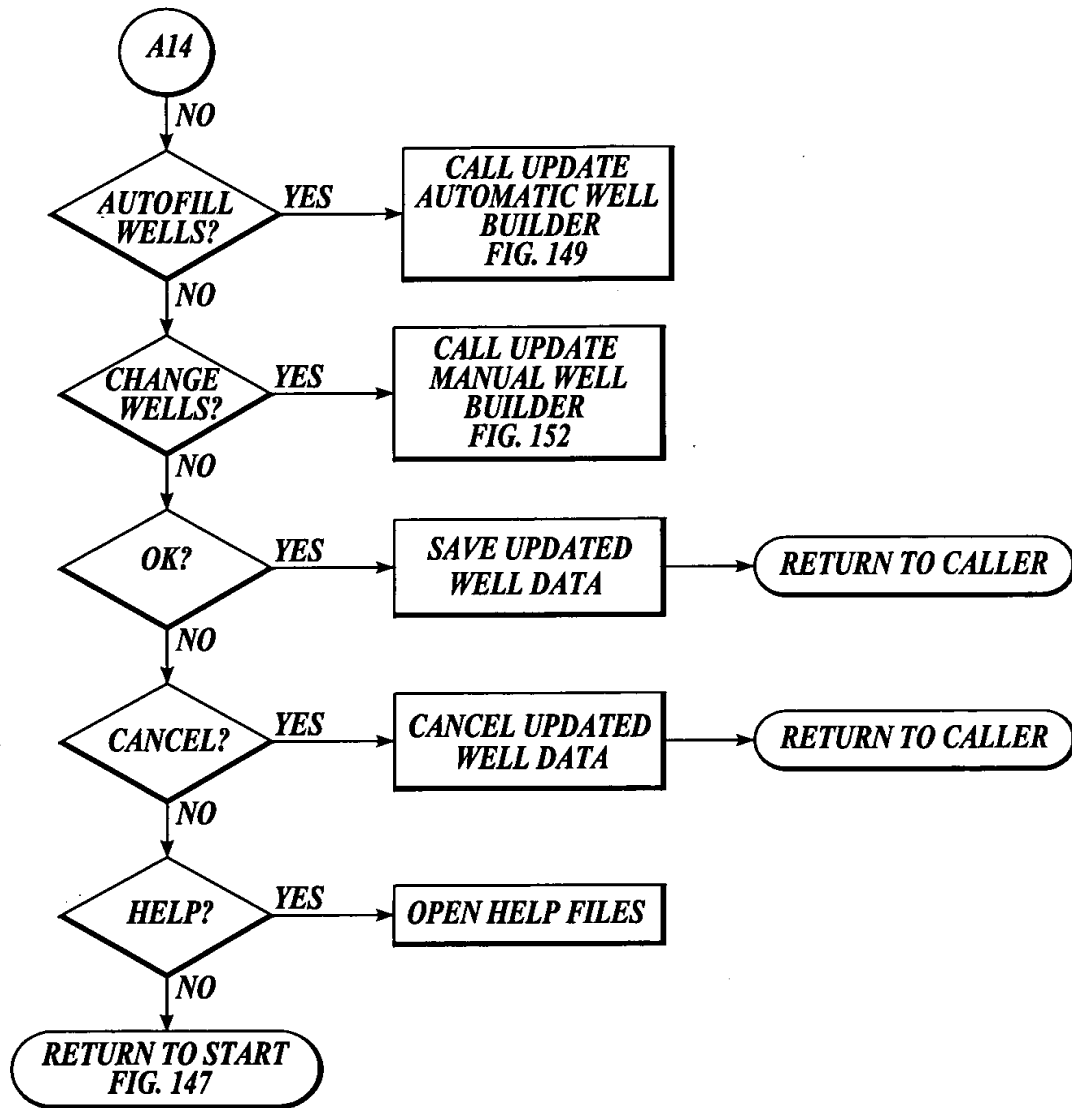


Fig. 147

**Fig. 148**

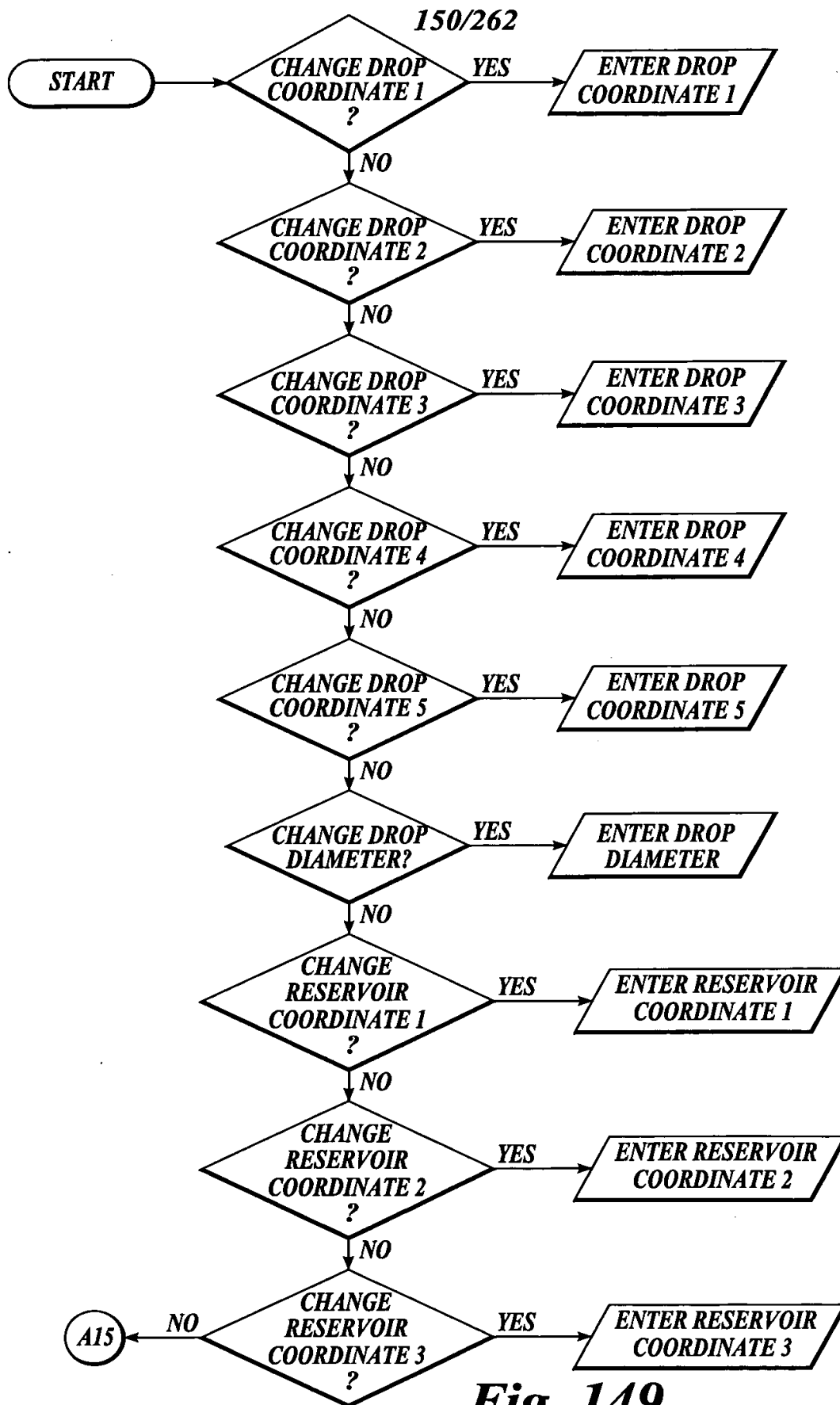
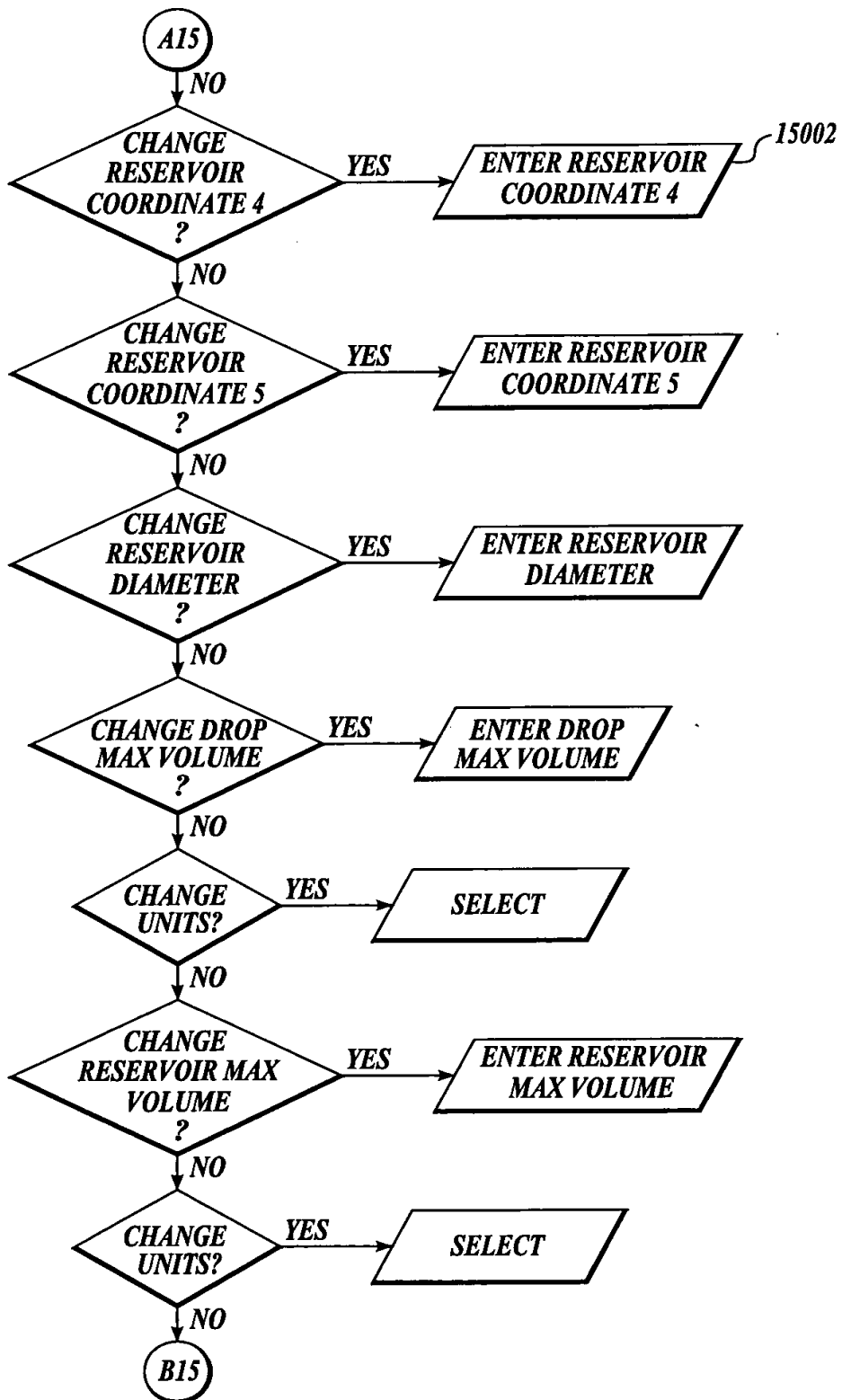
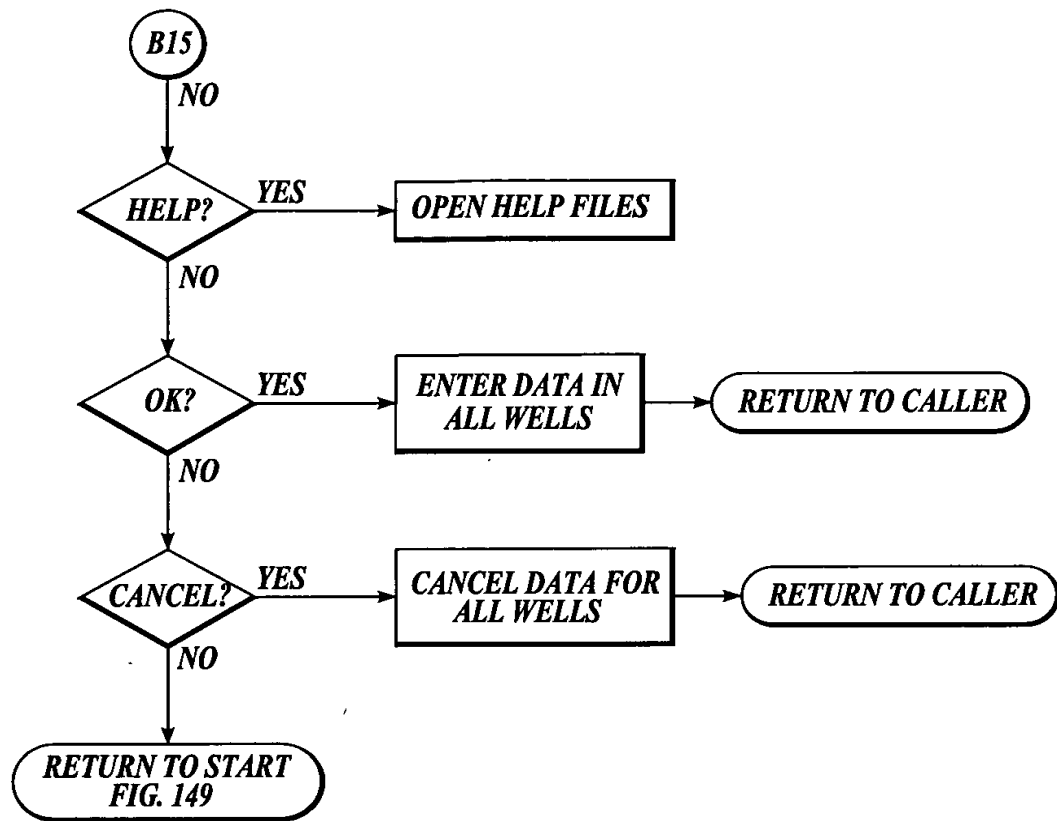
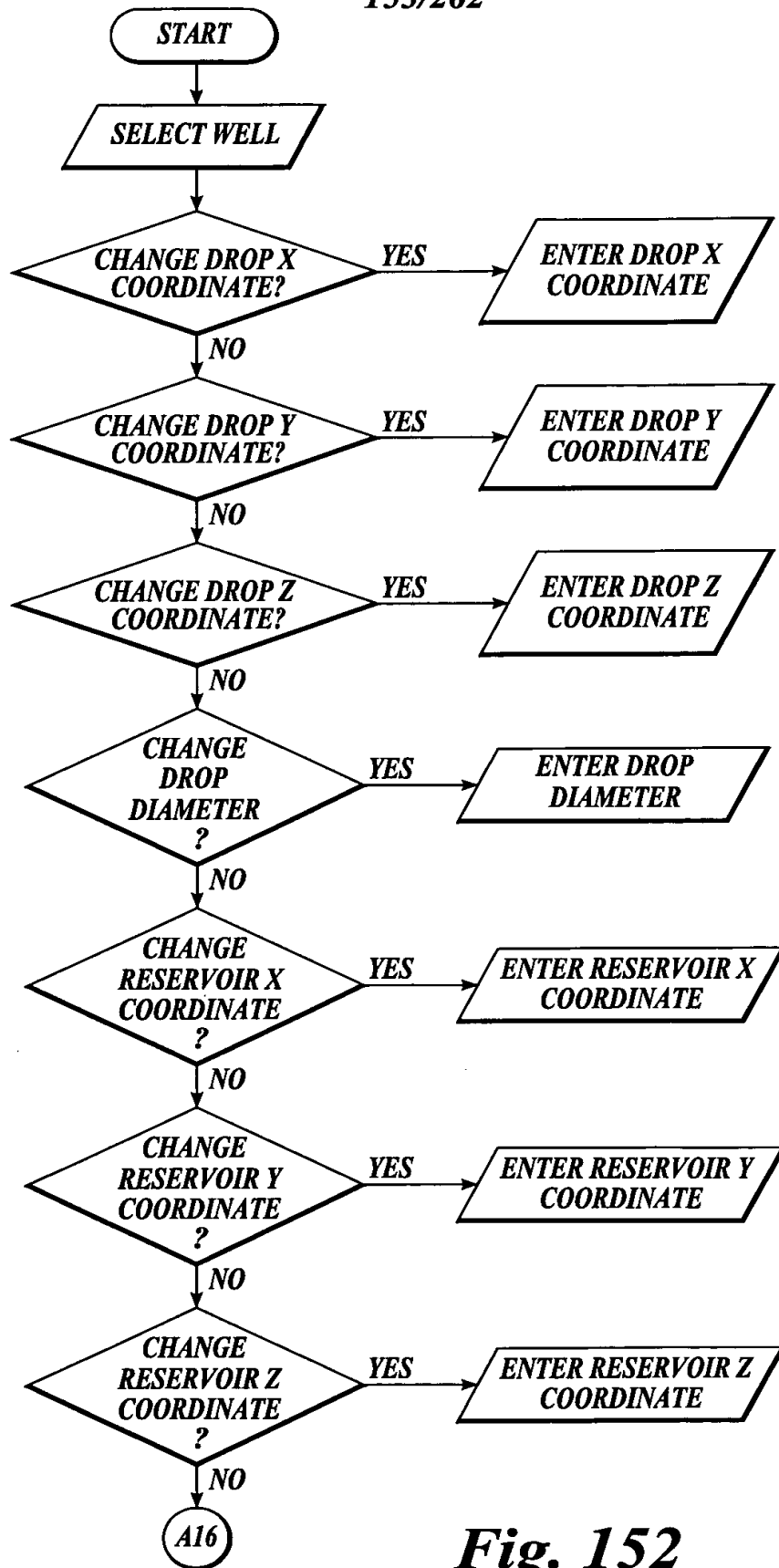
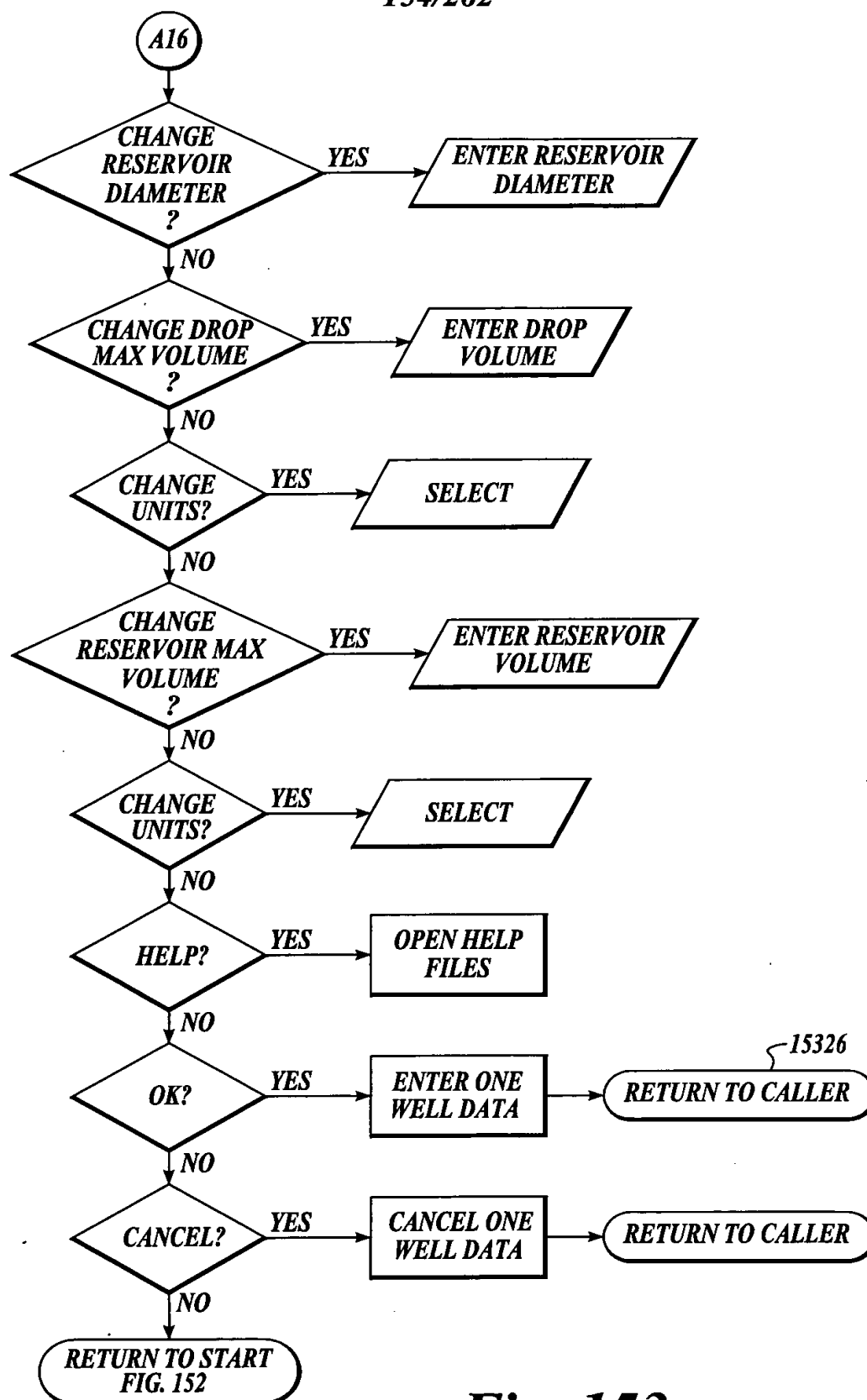


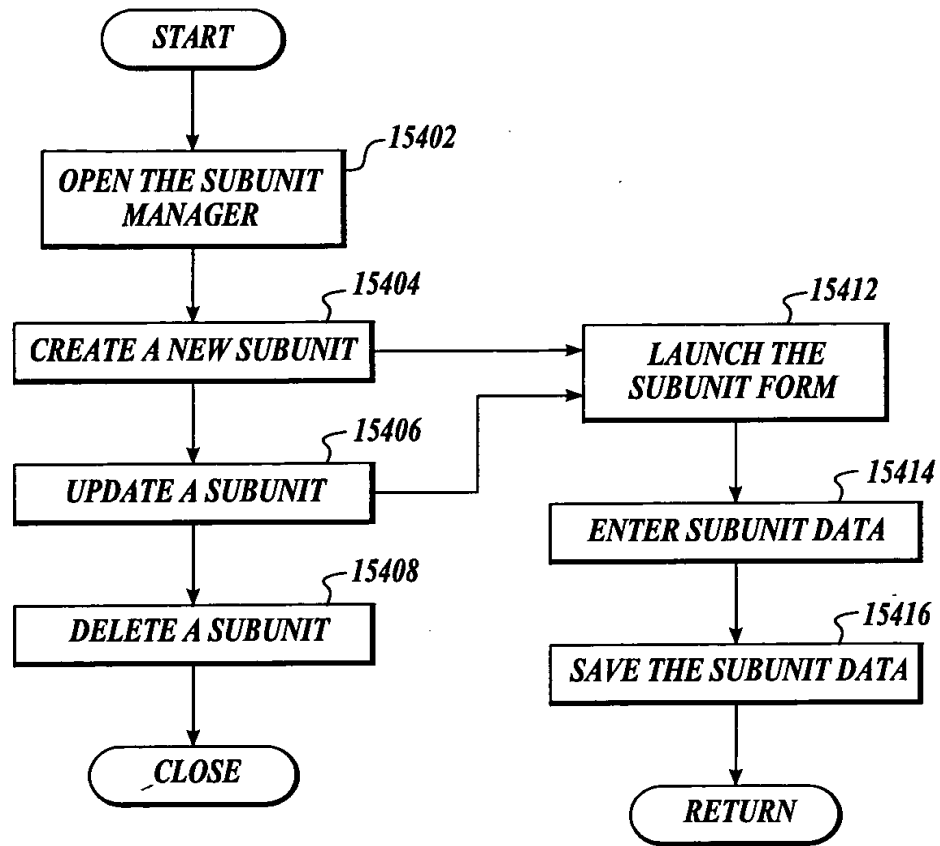
Fig. 149

**Fig. 150**

*Fig. 151*

**Fig. 152**

**Fig. 153**

*Fig. 154*

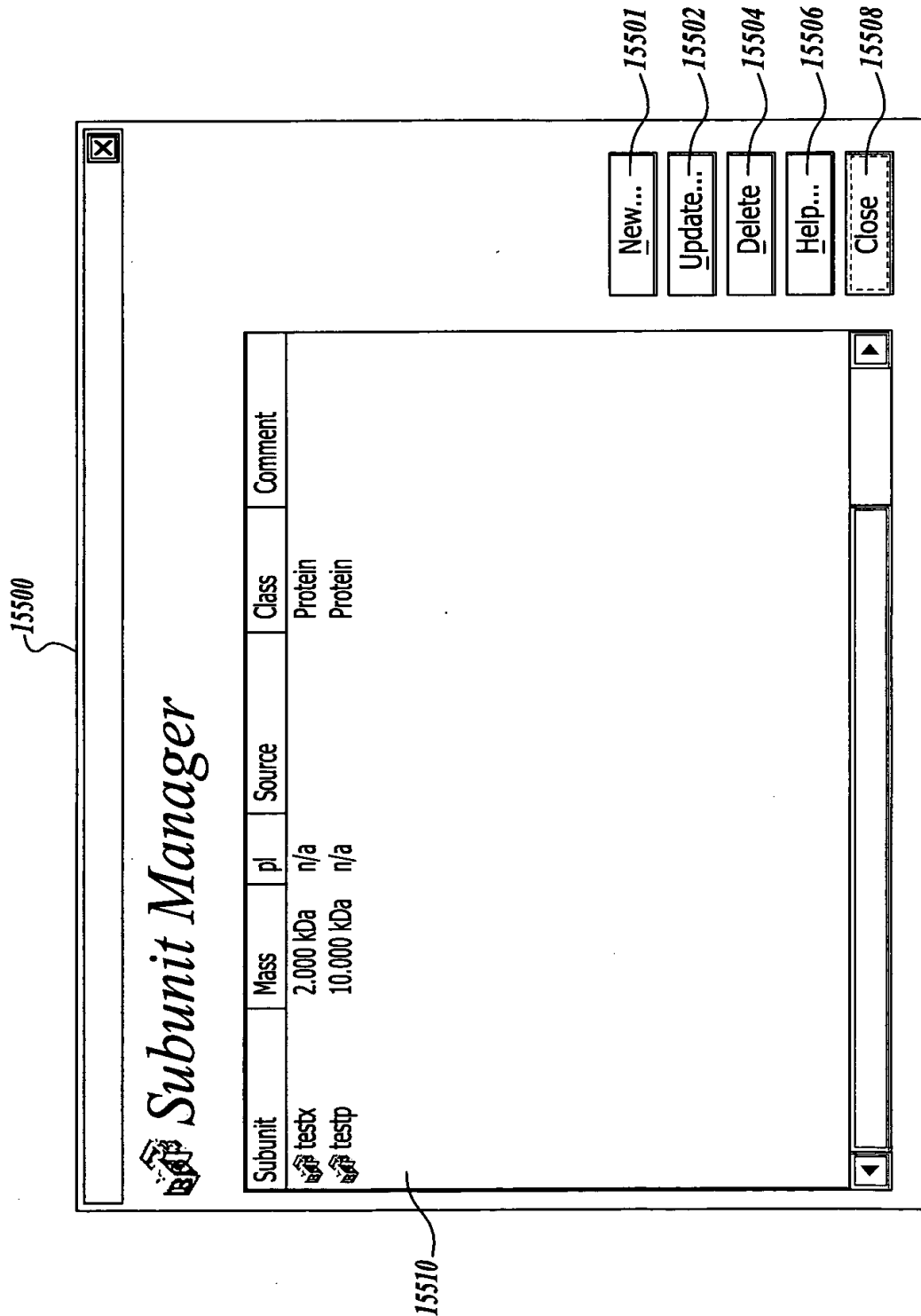
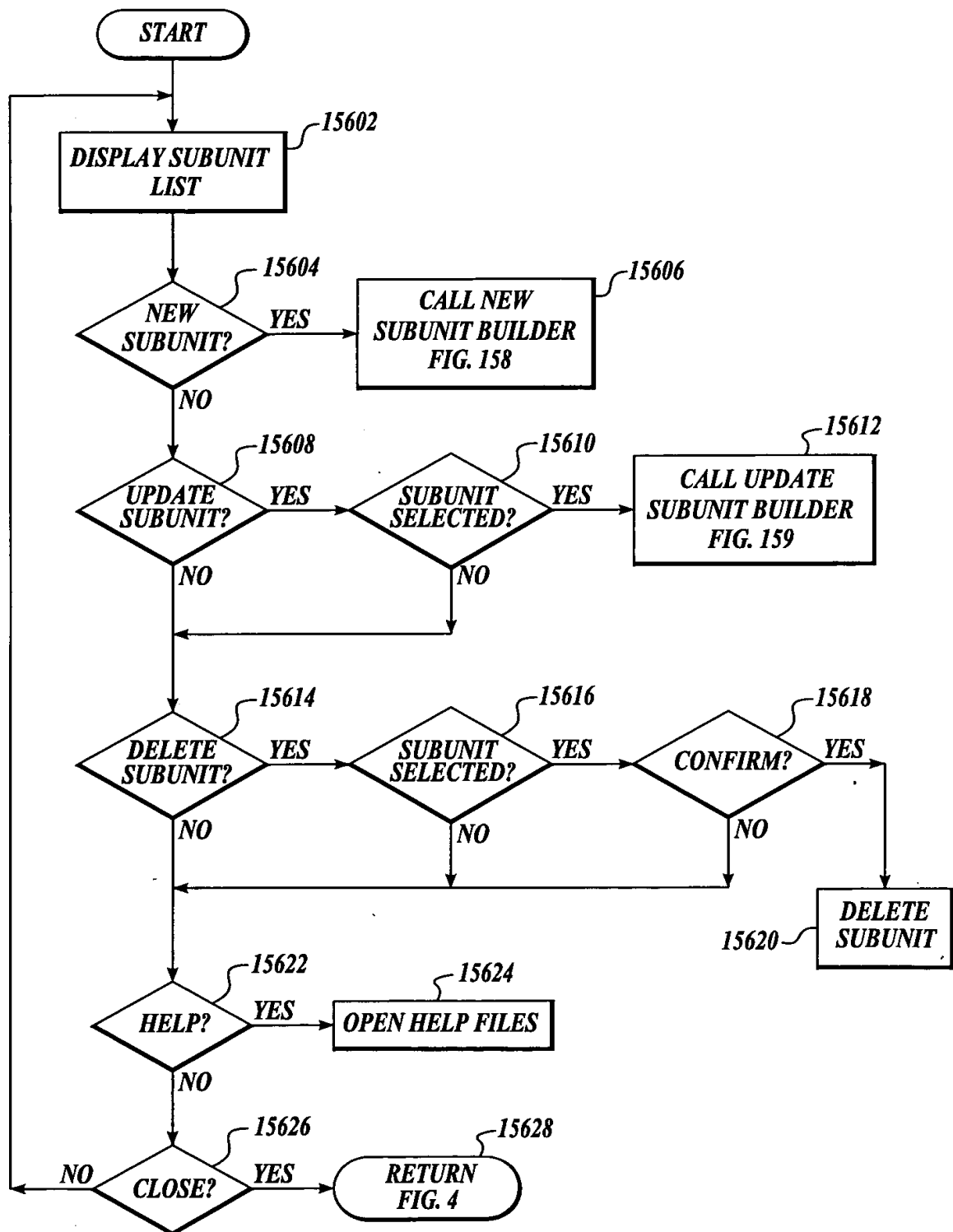


Fig. 155

**Fig. 156**

15700

New Subunit

Attributes

Name: 15701 TbGAPDH

Source: 15702 Trypanosoma brucei

15704 Class Name: 15706 Protein

Mass: 15710 40 15712 kDa

15708 pI: 15714

Comment: 15716 Trypanosoma brucei
glyceraldehyde-3-phosphate
dehydrogenase

OK 15718 Cancel 15720

Fig. 157

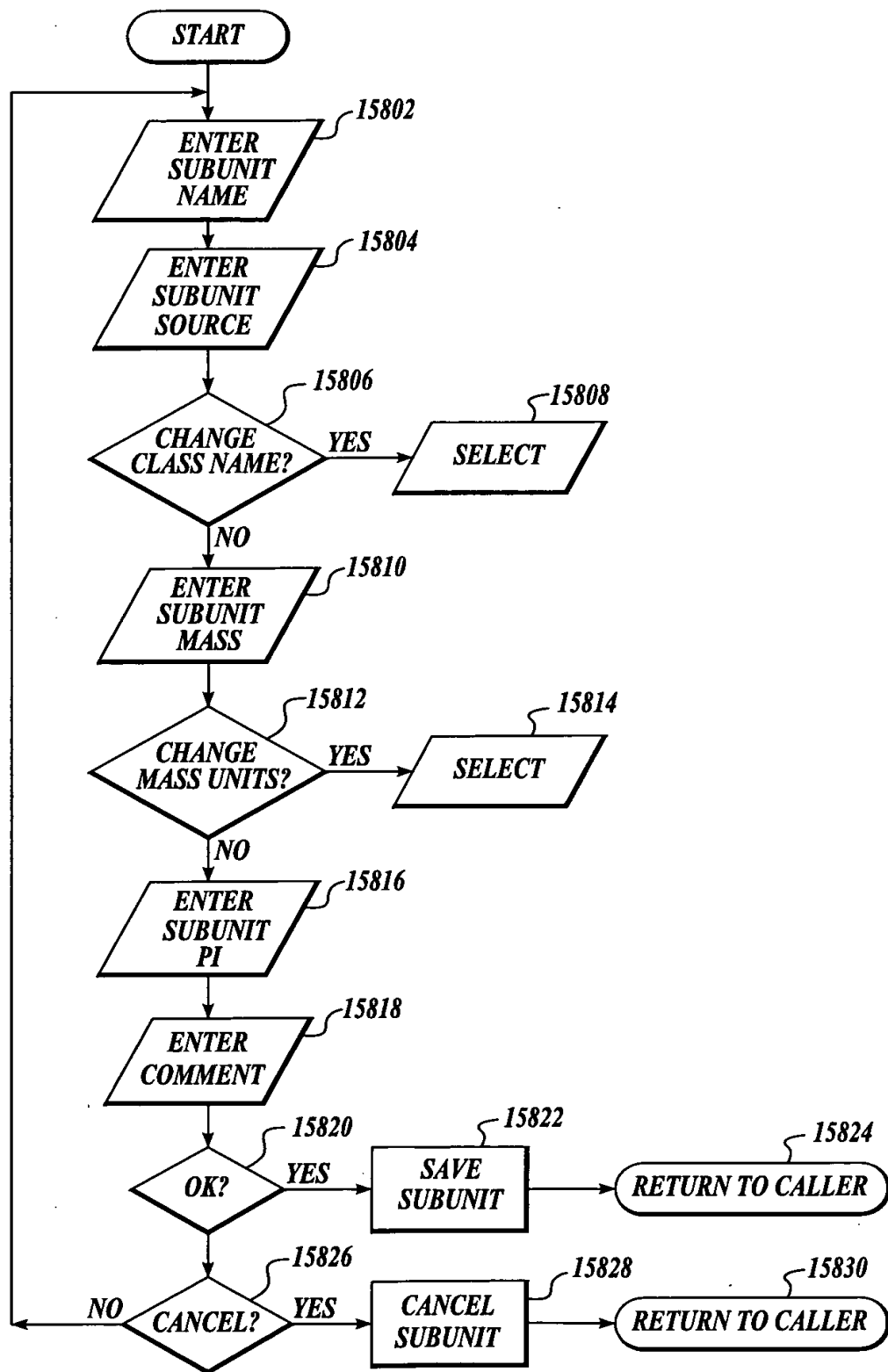
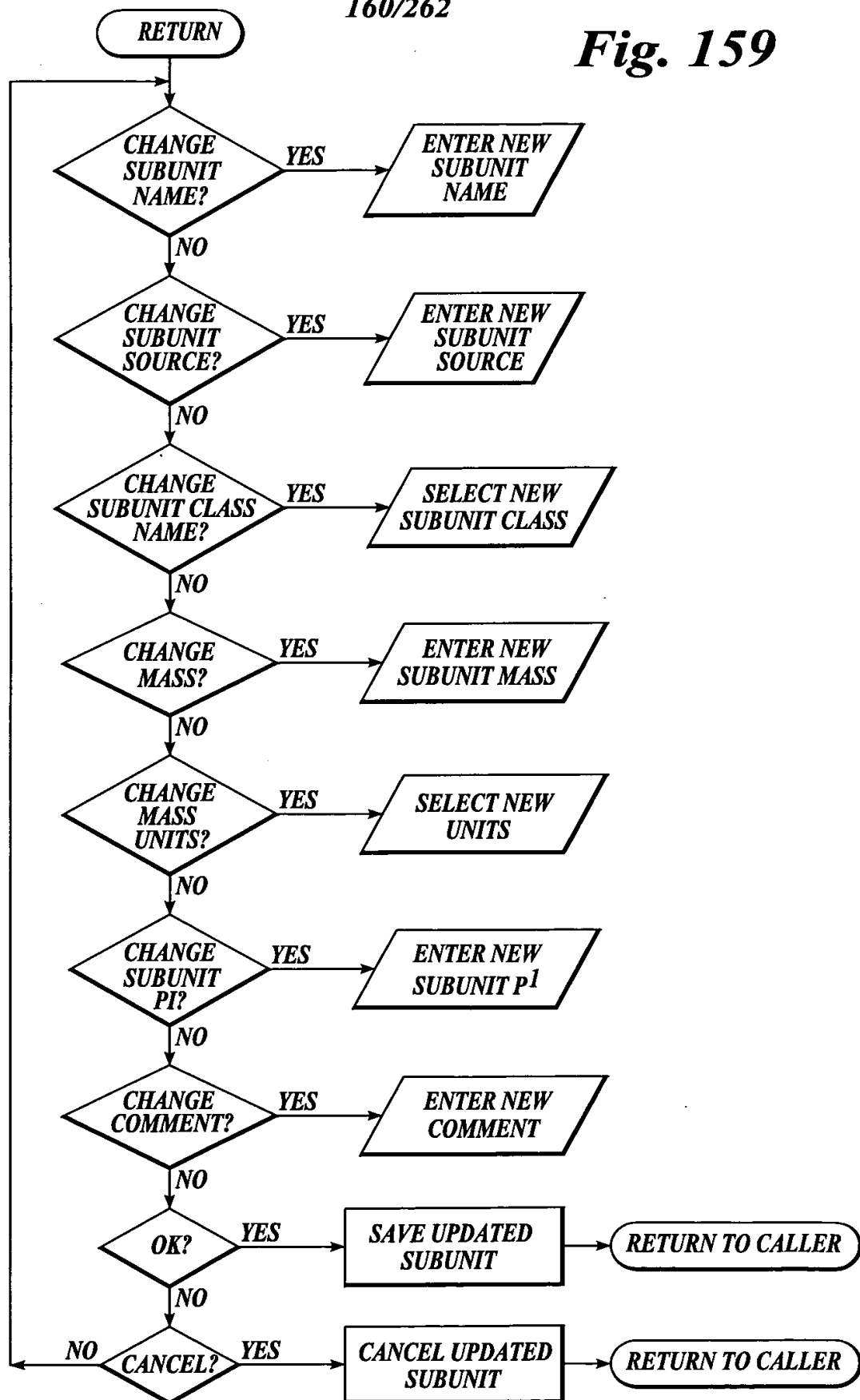
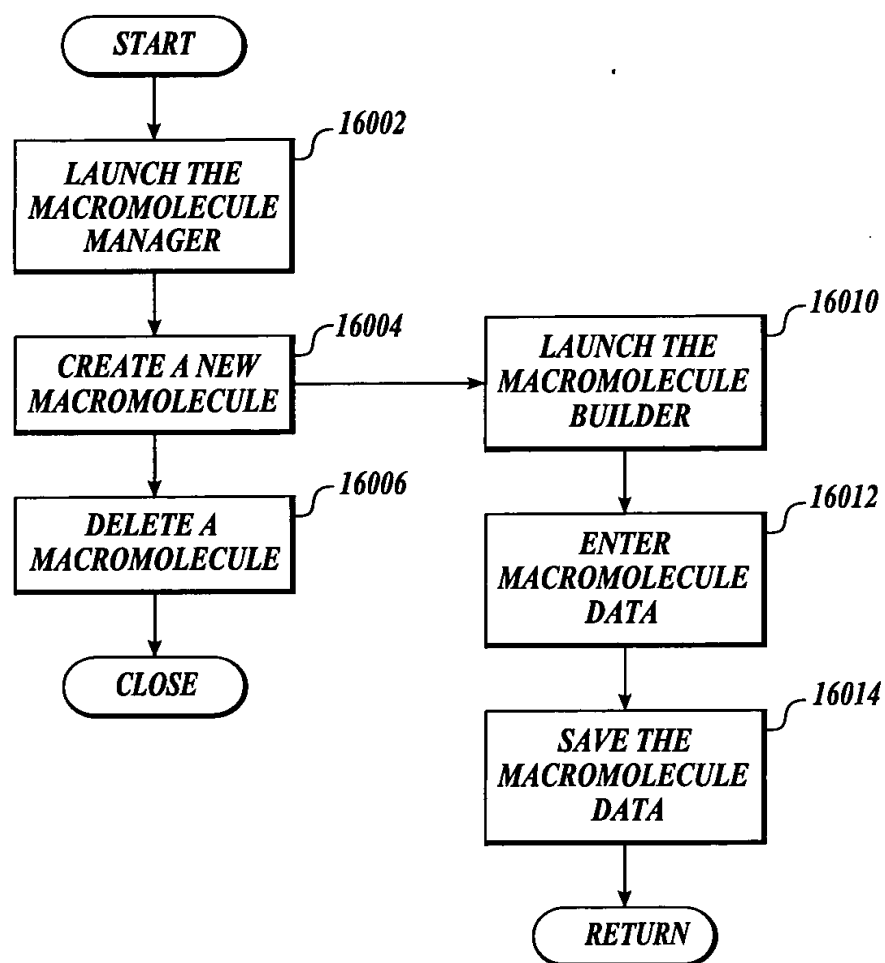
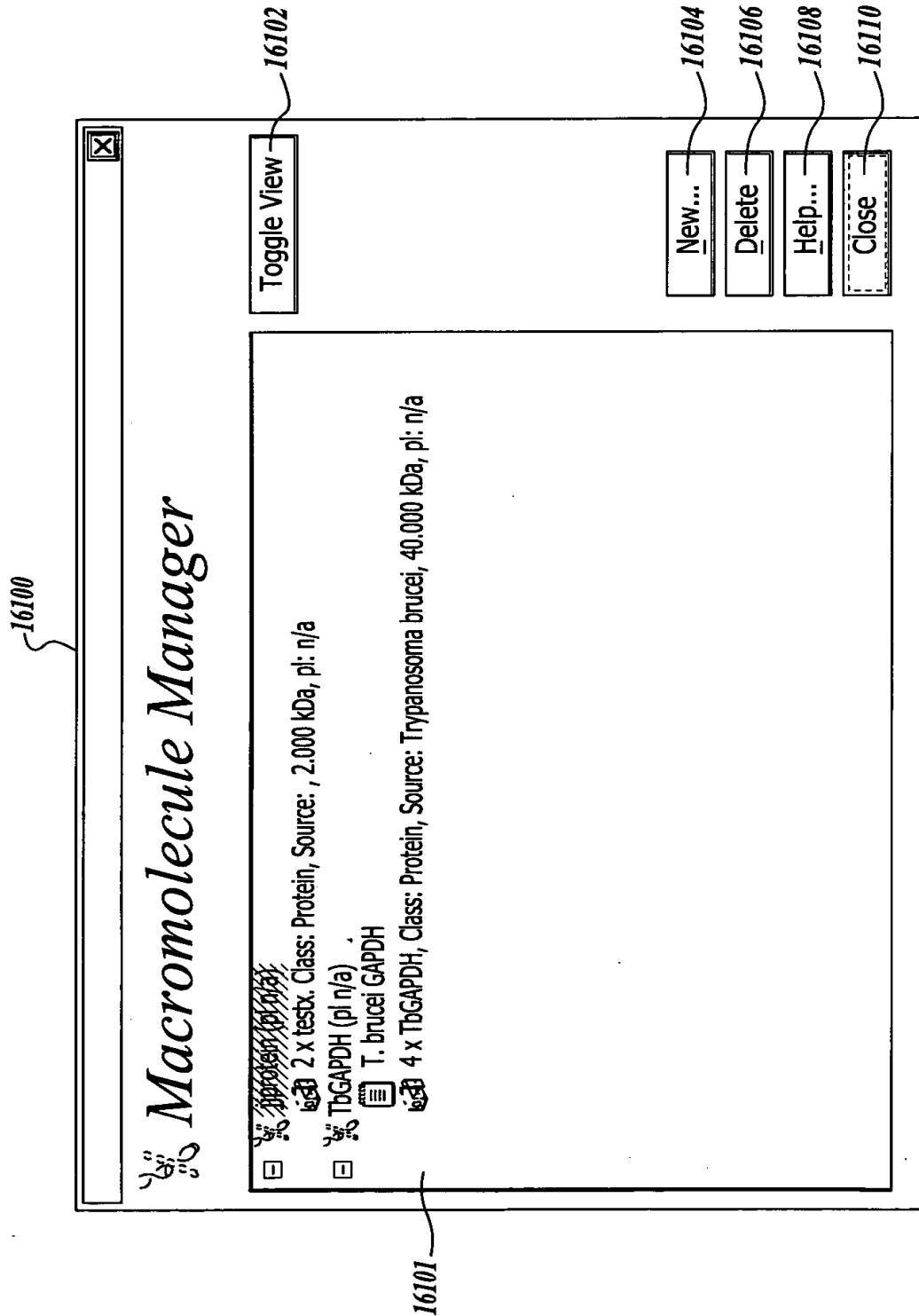
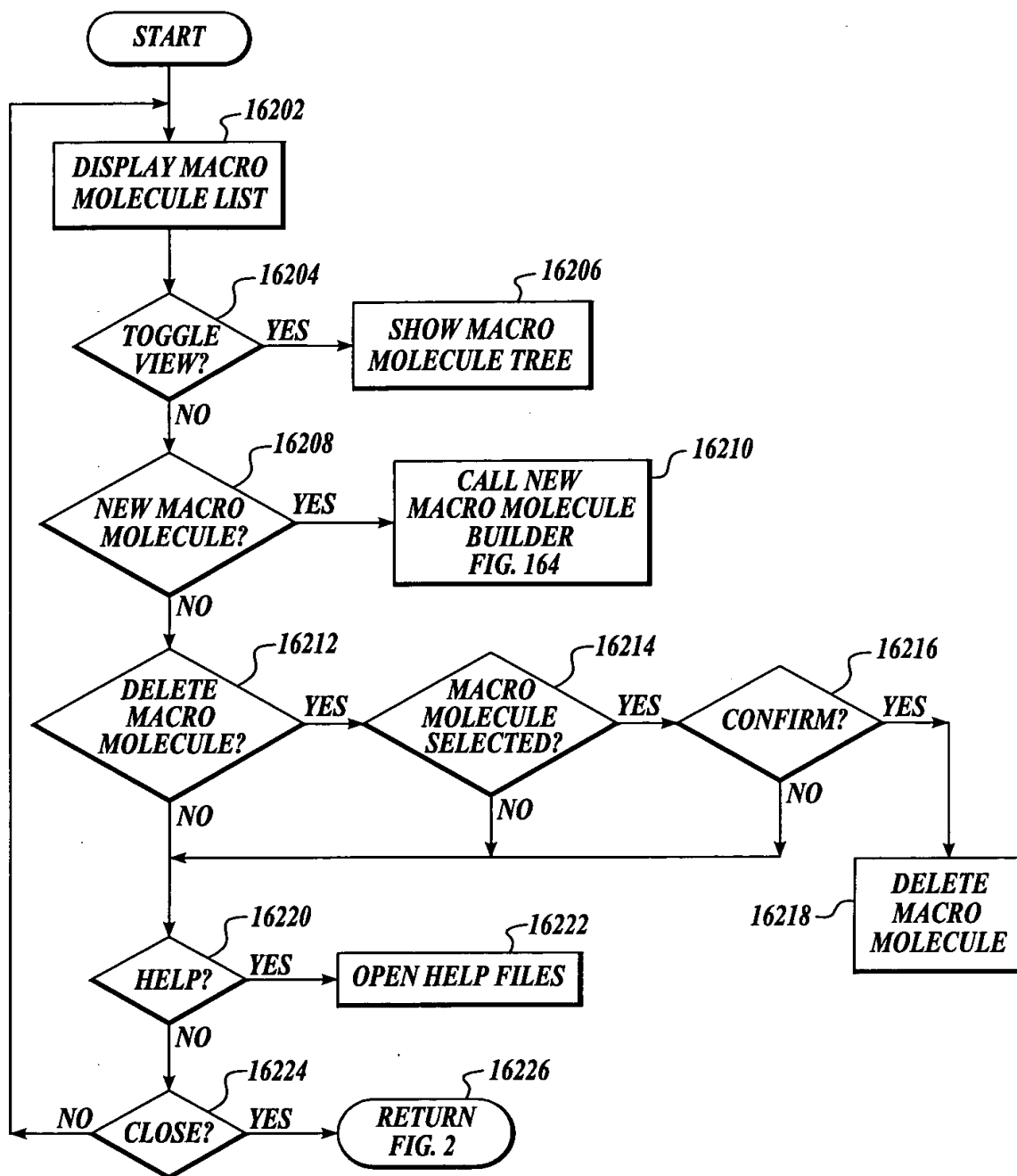
**Fig. 158**

Fig. 159

**Fig. 160**

*Fig. 161*

*Fig. 162*

16300

Macromolecule Builder

16304

Create Subunit...

Subunits:

Subunit	Mass	pI	Source
4testx	2.000 kDa	n/a	
testp	10.000 kDa	n/a	
TbGAPDH	40.000 kDa	n/a	Trypan

16301

Molecule Name: 4testx 16312

pI: 16314

Molecule Class: Protein 16316

Comment: testx holo-tetramer 16318 16320

Subunits associated with new Molecule:

Count	Subunit	Mass	pI	Source
4	testx	2.000 kDa	n/a	

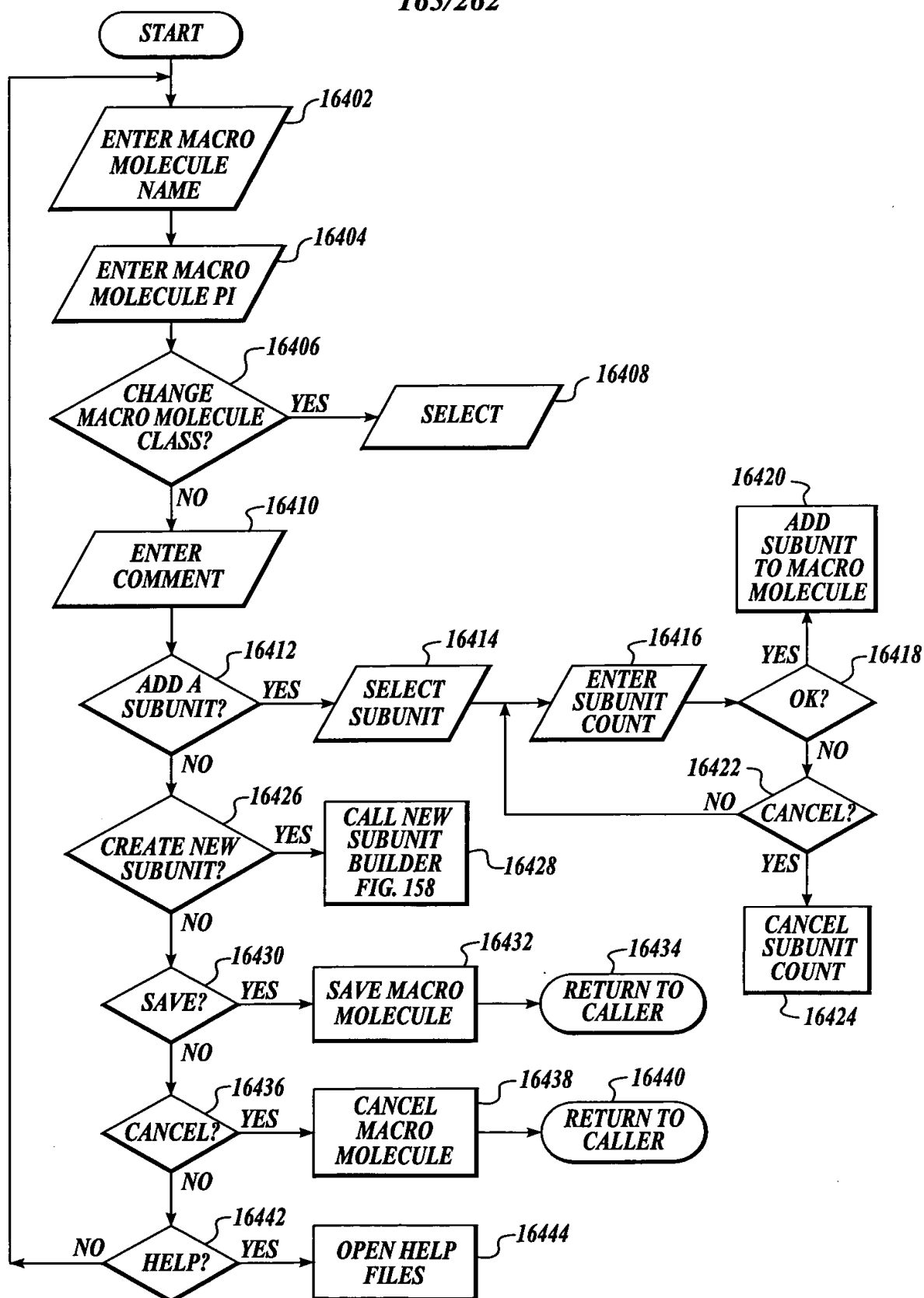
16302

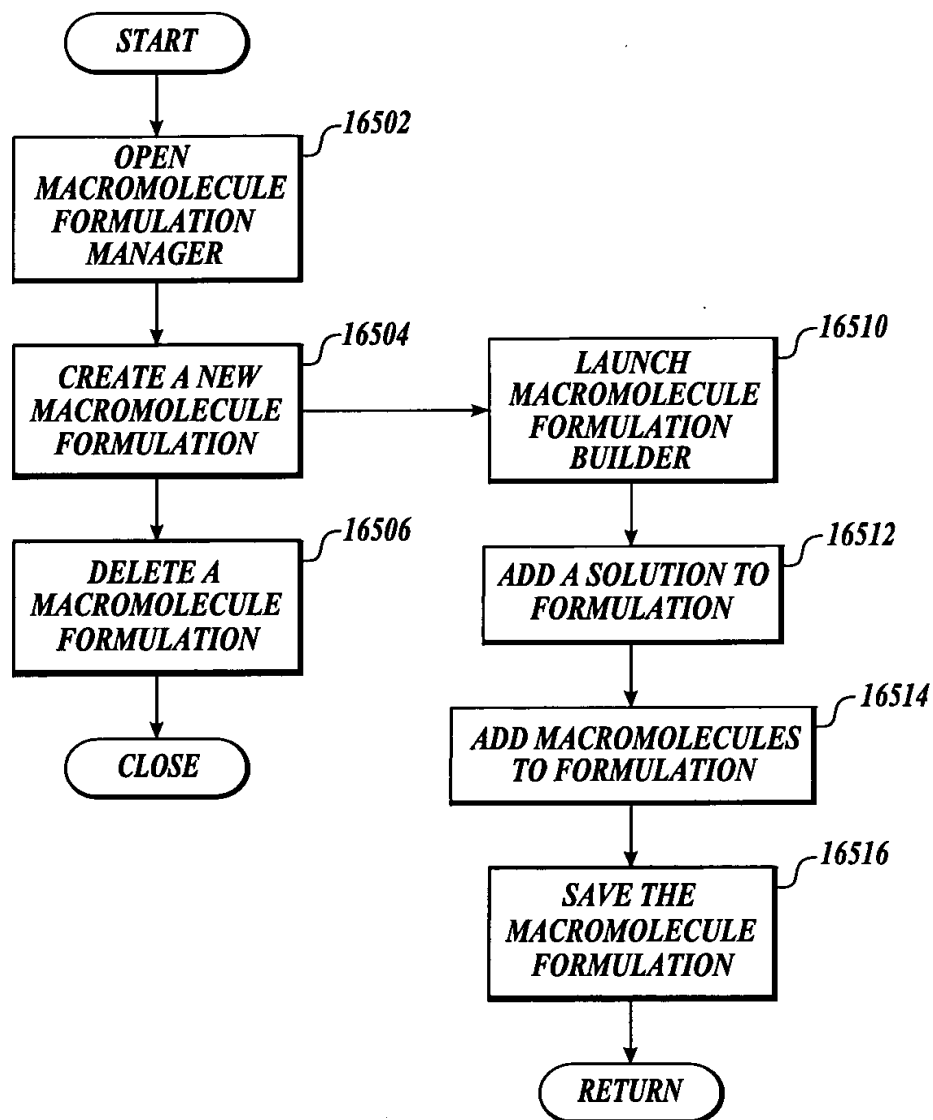
16306

Cancel 16308

Help... 16310

Fig. 163

**Fig. 164**

*Fig. 165*

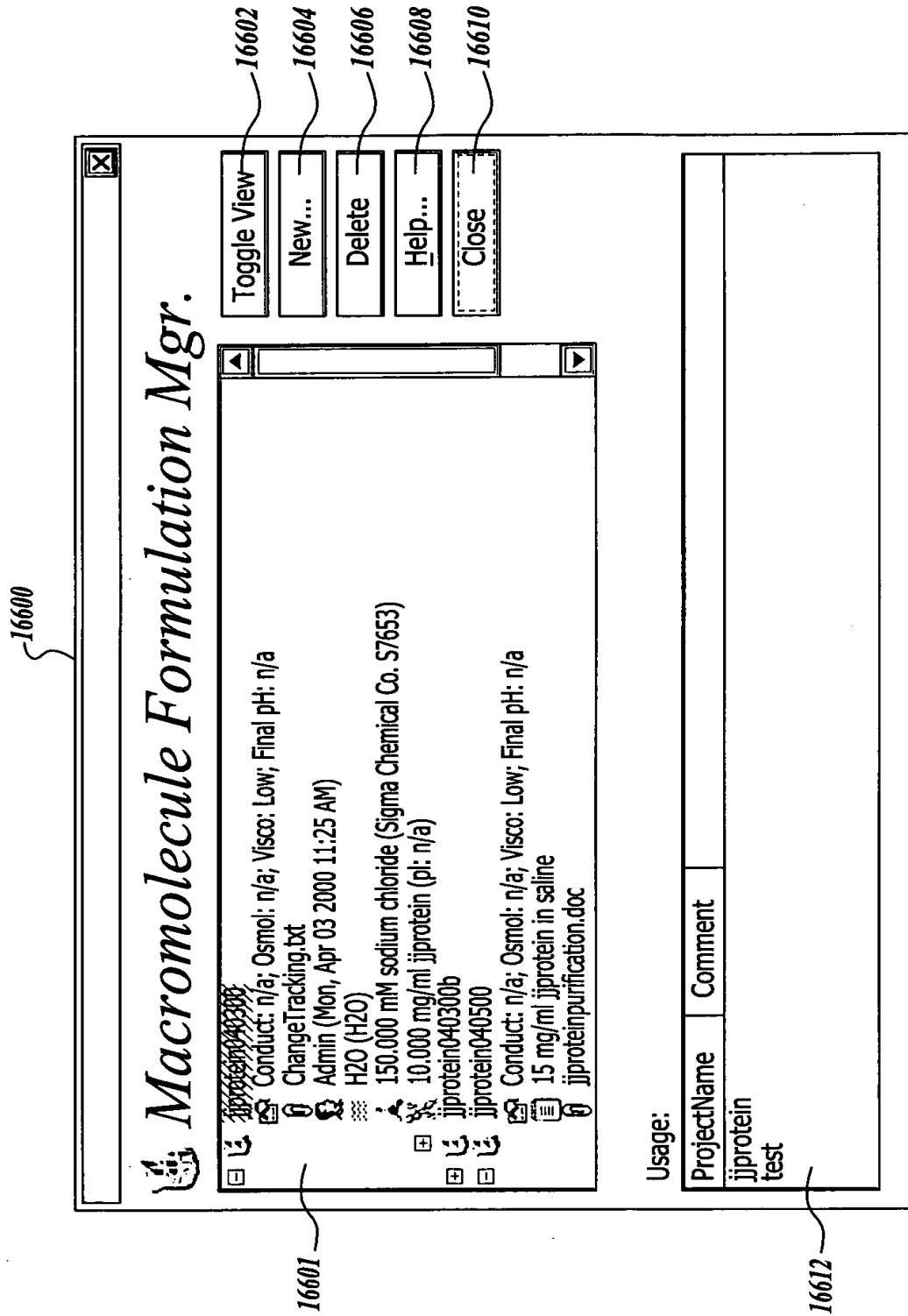
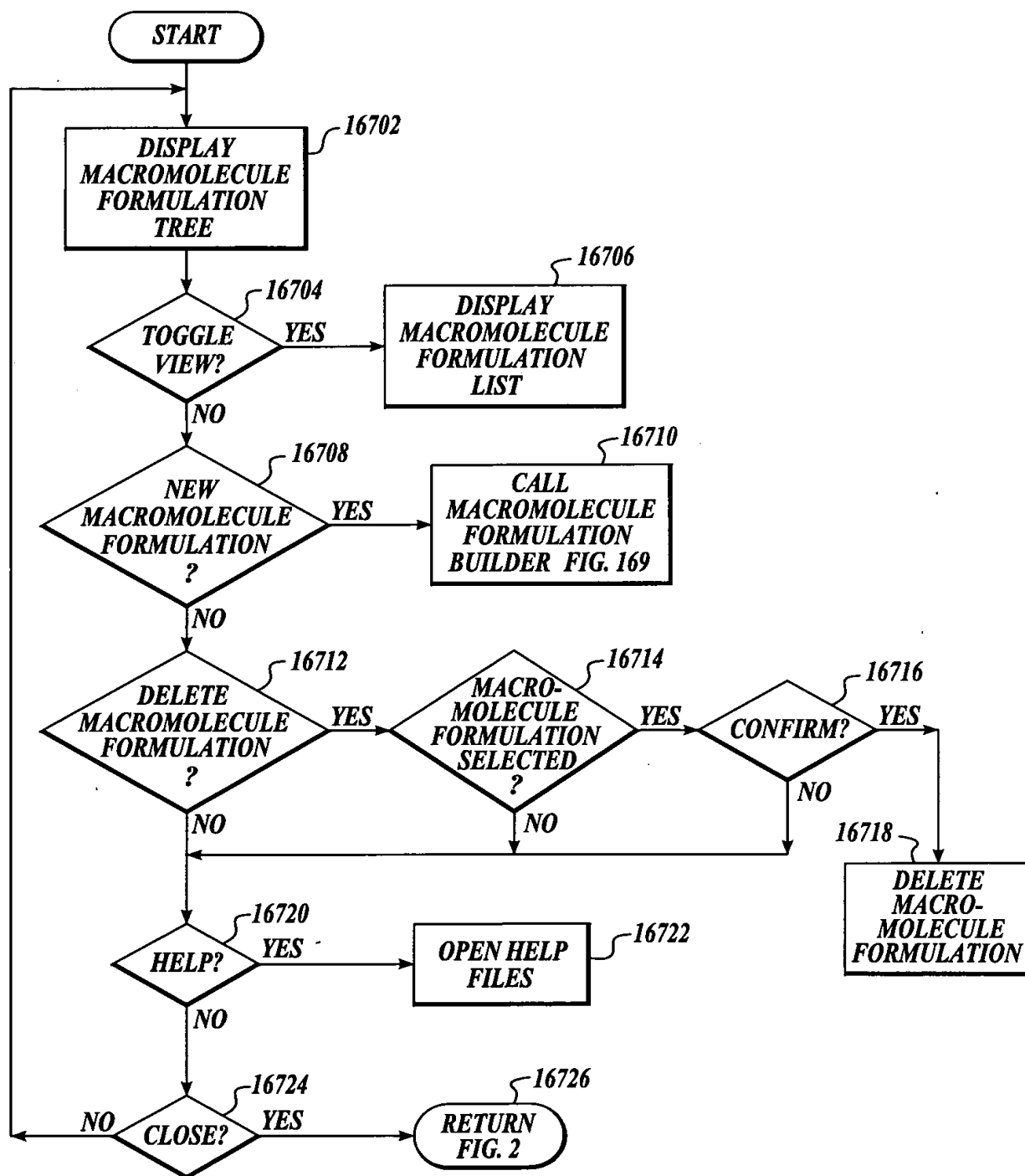


Fig. 166

**Fig. 167**

16802

Macromolecule Formulation Builder

16808

Solutions Macromolecules

New Macromolecule...

4testx (pl n/a)
 4 x testx, Class: Protein, Source: , 2,000 kDa, pl: n/a
 augx (pl n/a)
 2 x testx, Class: Protein, Source: A. vinelandii, 34.00
 ijprotein (pl n/a)
 2 x testx, Class: Protein, Source: , 2,000 kDa, pl: n/a
 TbGAPDH (pl n/a)
 4 x TbGAPDH, Class: Protein, Source: Trypanosoma

16804

Molecule List:

15.000 mg/ml 4testx

16806

Solution: saline

16801

Prep. Date: 4/ 7/00

16812

Storage Temp: Protein C

16810

Preparator: Admin

16818

Macromolecule Formulation Name: ijprotein040700

16816

16822

16820

16814

16824

E:\cymon\Help\crystalmonitor\images\ijprot

16825

Comment:

15 mg/ml ijprotein in saline

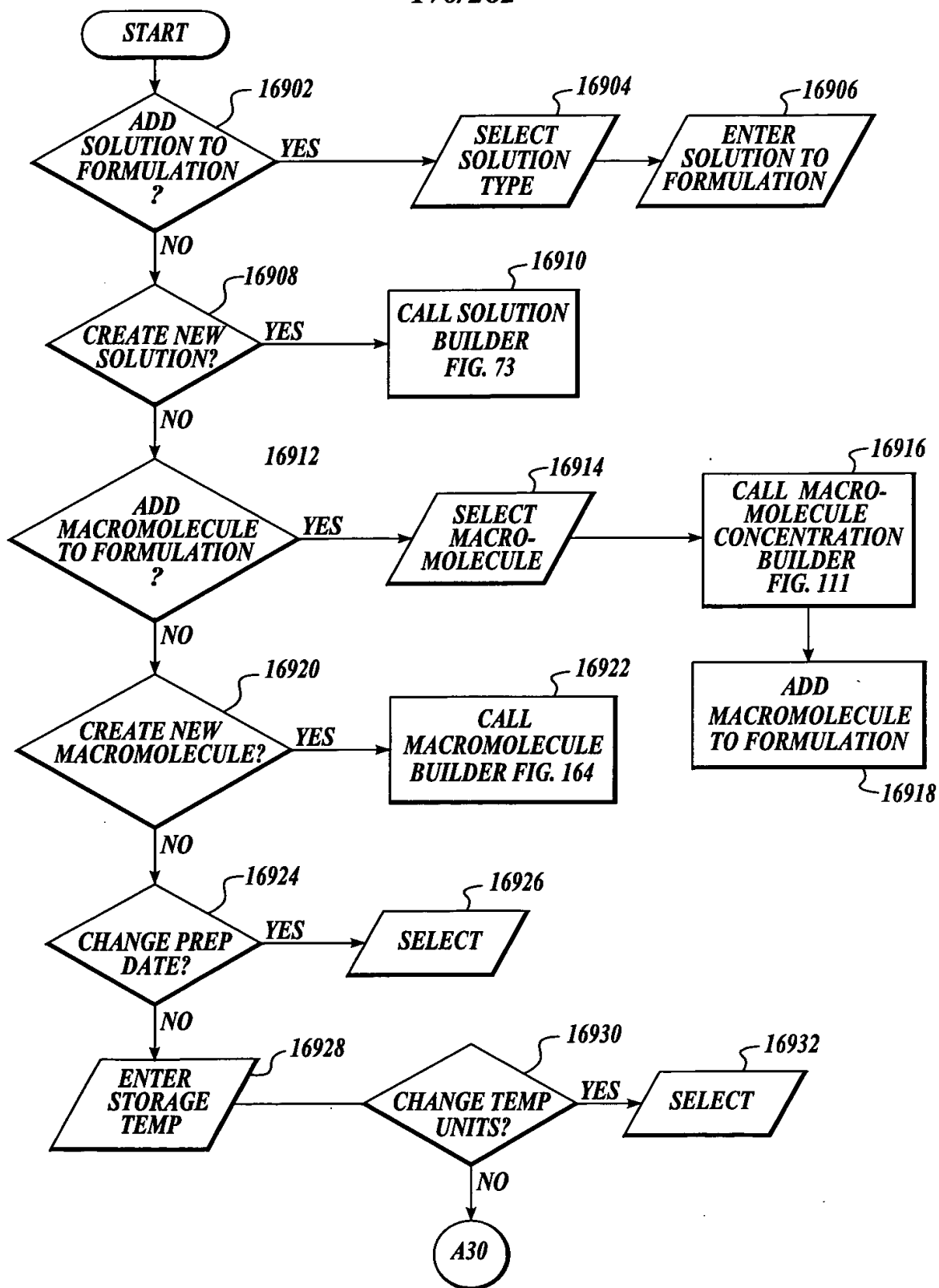
16827

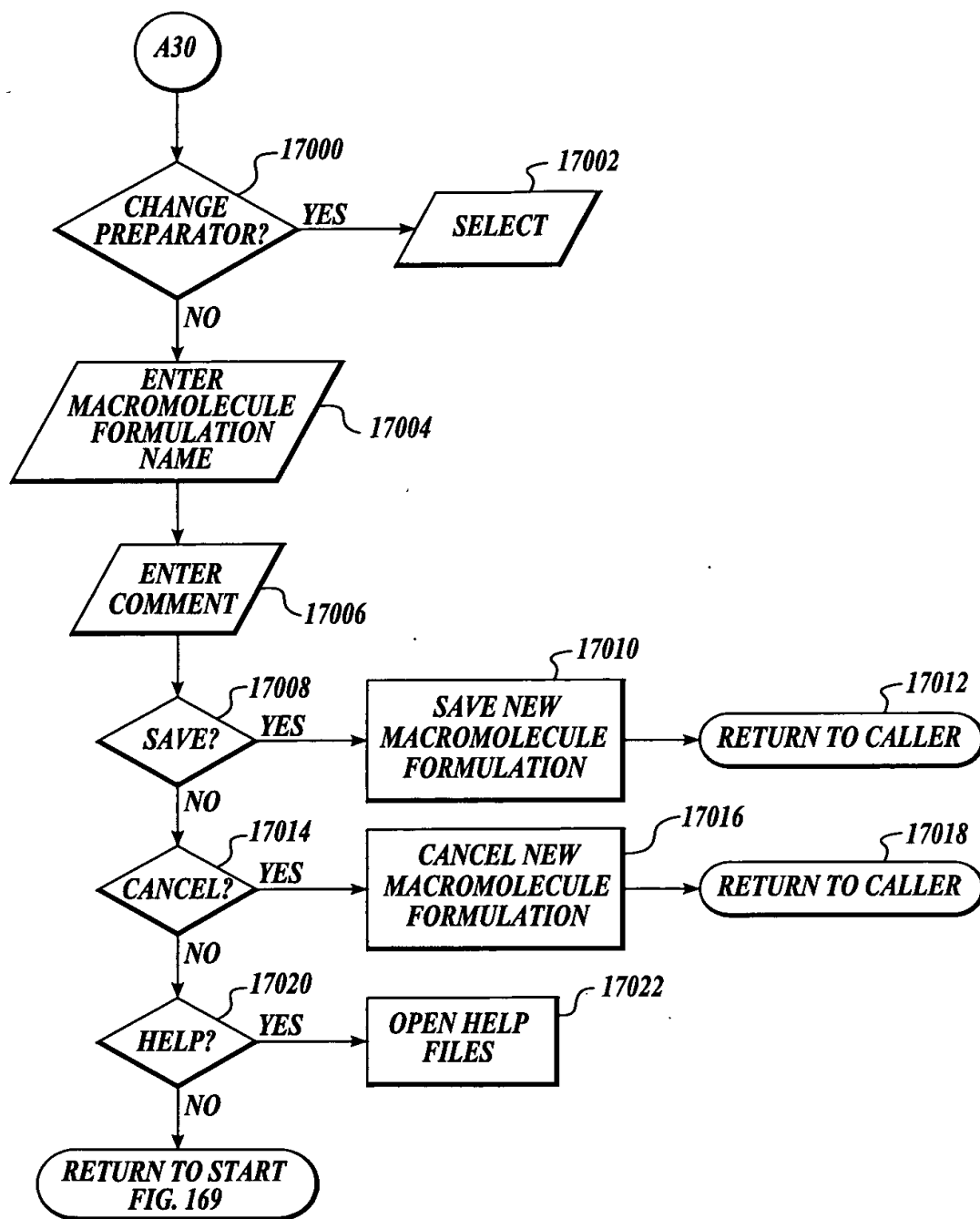
16826

16828

16830

Fig. 168

**Fig. 169**

**Fig. 170**

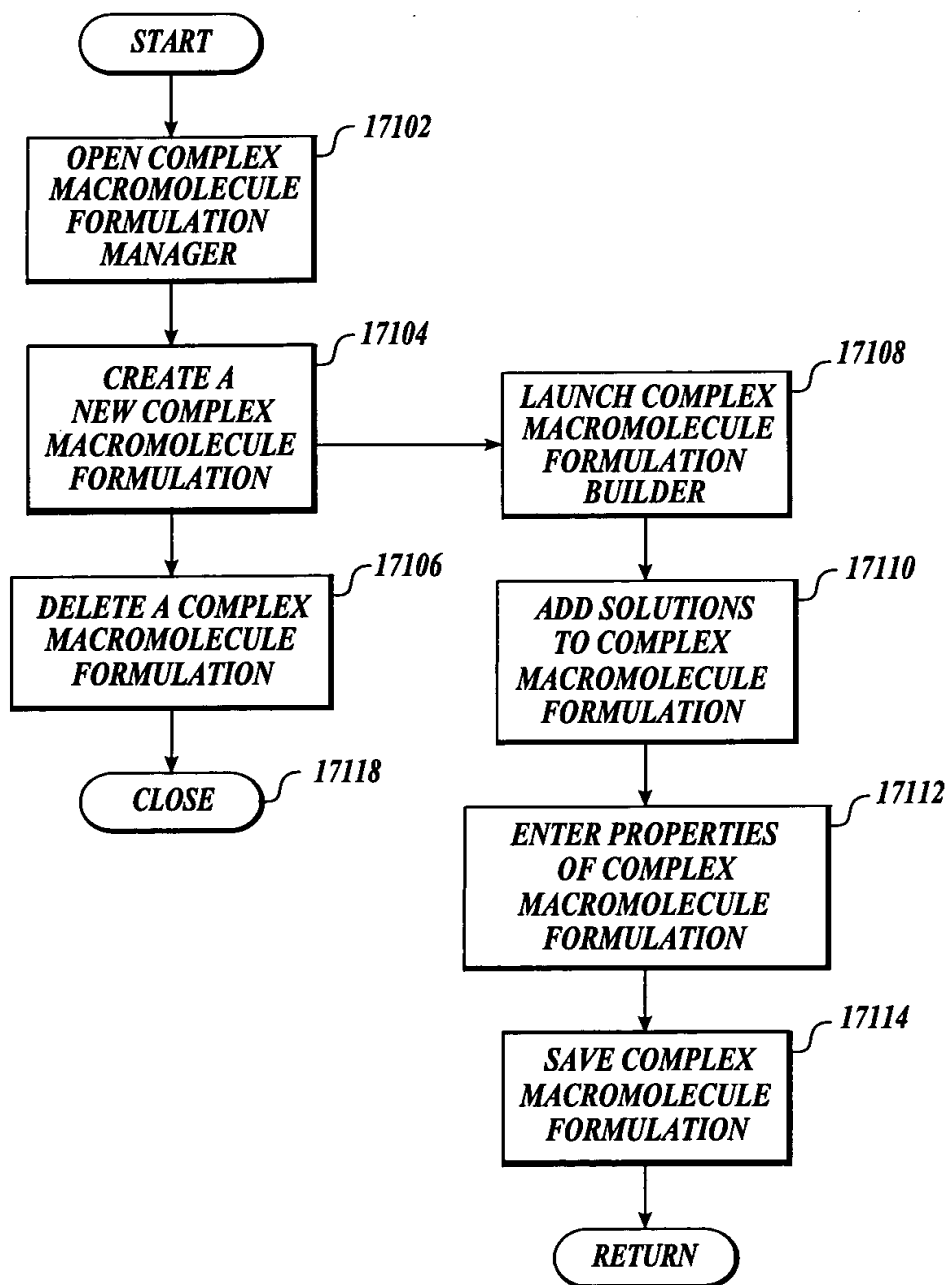
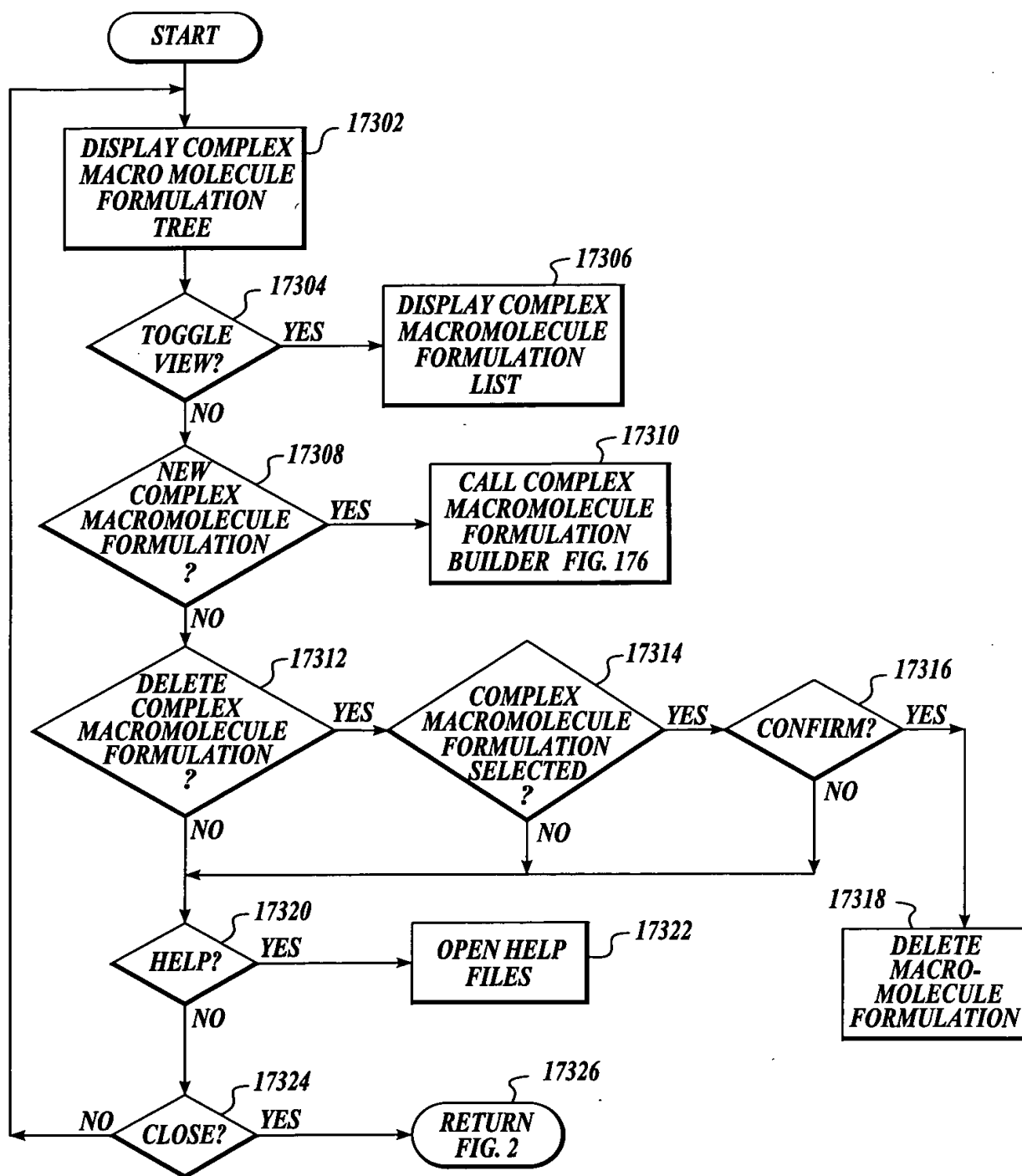
*Fig. 171*



Fig. 172

*Fig. 173*

Complex Molecule Formulation Builder

17401 Solutions 17408 Properties 17402

17404

17410

☐ Additive
☐ Formulation
☐ HeavyAtom
☐ Buffer Solution
☐ Stock Solution
☒ Macromol. Form.
☐ Cplx. Macromol.

Toggle

ijprotein040300 Conduct: n/a; Osmo
 ChangeTracking.txt
 Admin (Mon, Apr 03
 H2O (H2O)
 150.000 mM sodium
 10.000 mg/ml ijprote
 ijprotein040300b
 Conduct: n/a; Osmo
 20 mg/ml ij protein in
 Admin (Mon, Apr 03
 H2O (H2O)
 150.000 mM sodium
 20.000 mg/ml ijprote
 ijprotein040500
 ijprotein040700

Final Complex Macromolecule Formulation:

500.000 µl ijprotein040300
 50.000 % H2O (H2O)
 75.000 mM sodium chloride
 5.000 mg/ml ijprotein (pl: n/a)
 500.000 µl ijprotein040700
 50.000 % H2O (H2O)
 75.000 mM sodium chloride
 7.500 mg/ml 4testx (pl: n/a)

Total Vol: 1000.000 µl

Fig. 174

17500

Complex Molecule Formulation Builder

17501 Solutions Properties 17502

17503 Timestamp: 4/ 7/00 17504

17505 Storage Temp: 4 17506

17507 Preparator: Admin 17508

17509 Final pH: 17510

17511 Conductivity μS/cm 17512

17513 Vapor Pressure Osmolality: mmole/kg 17514

17515 Solvent: H2O (Mothe) 17516

17517 New Solution Name: ijproteincomplex37 17518

17519 Viscosity: Low High 17520

17521 Comment: mix ijprotein040300 and ijprotein040700 17522

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17537

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17544

Fig. 175

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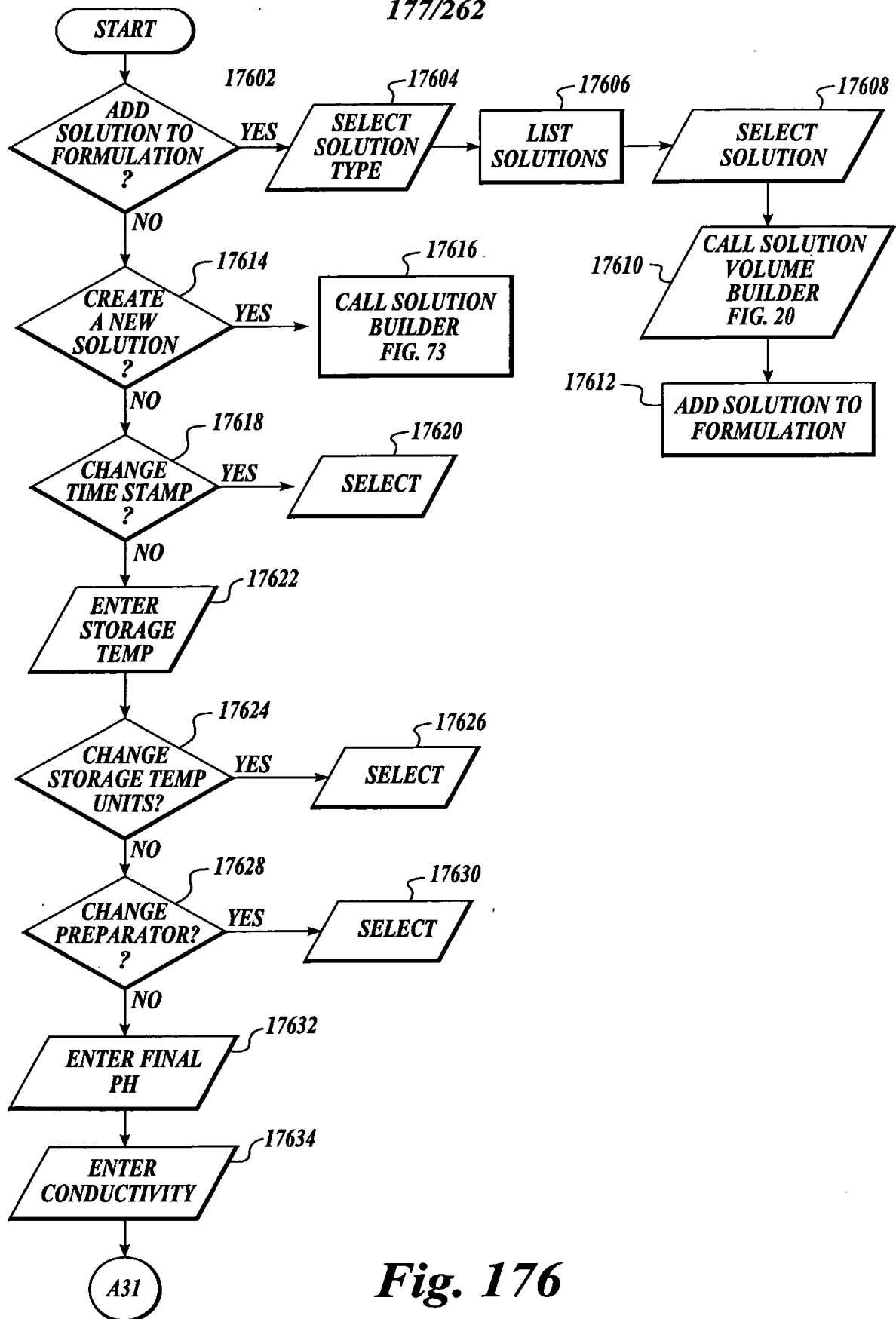


Fig. 176

178/262

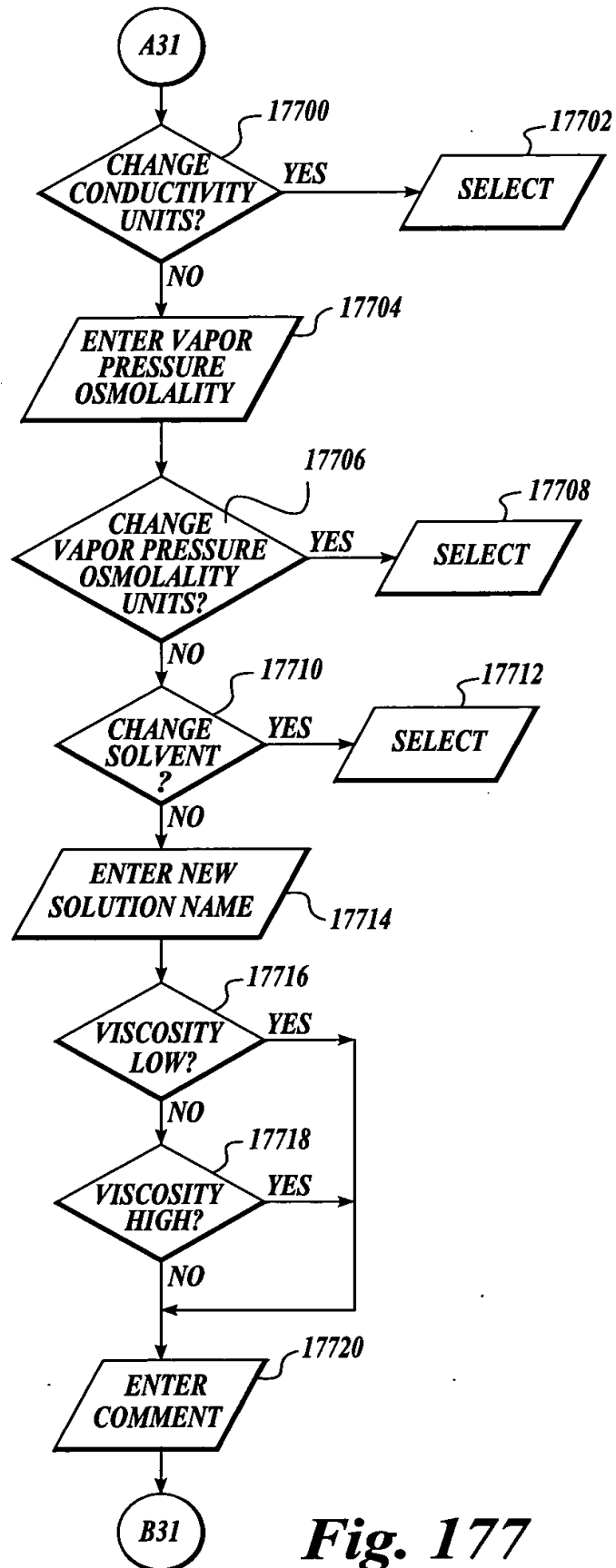
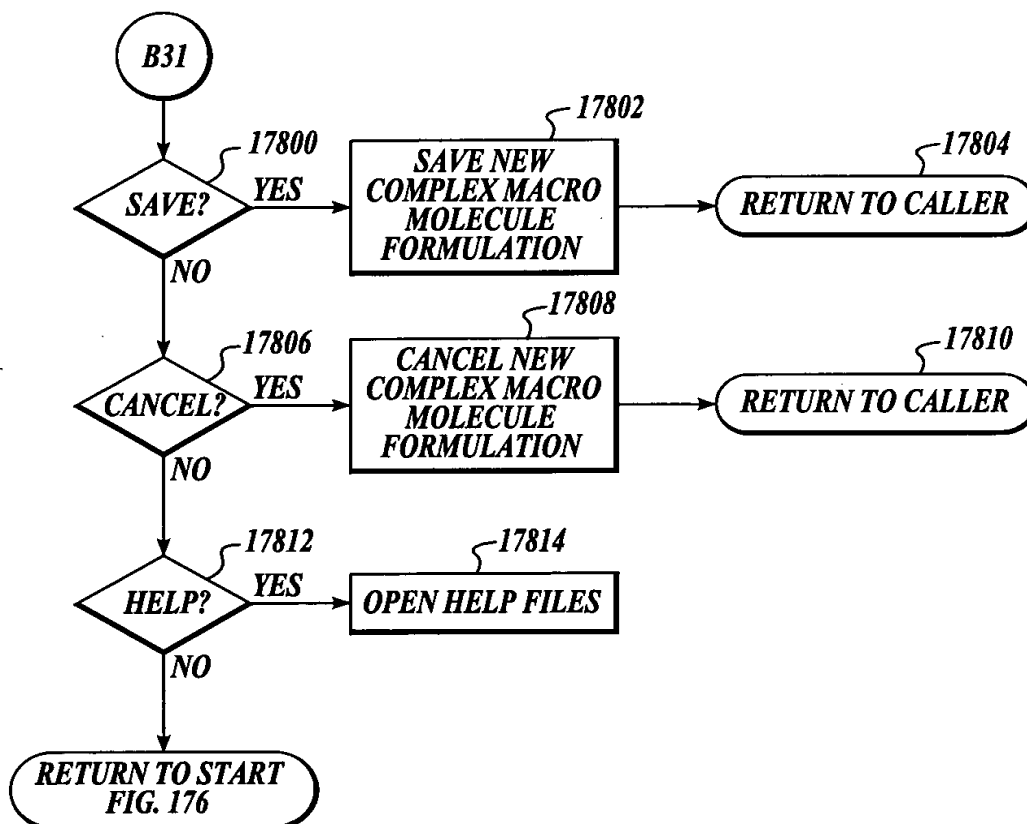
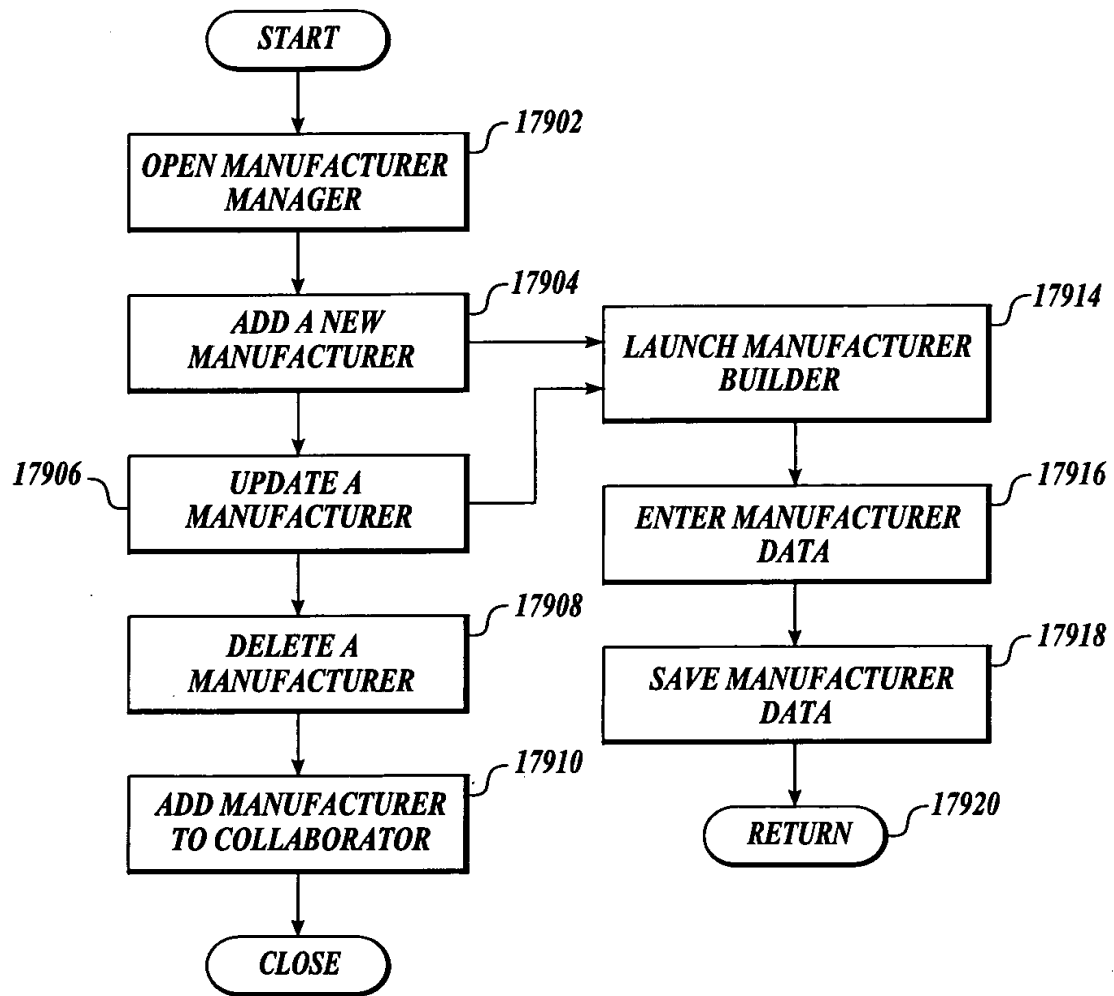


Fig. 177

**Fig. 178**

**Fig. 179**

Manufacturer Manager

Name	Phone	Street	City
Mother Earth	(800) 123-4567	Atmosphere and...	Milky Way
Emerald BioStructures, Inc.	(888) 780-8535	7865 NE Day R...	Bainbridge Isla
Sigma Chemical Co.	(800) 325-3010	P.O. Box 14508	St. Louis
Fluka Chemical Corp.	(800) 358-5287	1001 W St. Paul...	Milwaukee
Aldrich Chemical Co.	(800) 558-9160	P.O. Box 2060	Milwaukee
Fisher Scientific Co.	(800) 766-7000	585 Alpha Dr.	Pittsburgh
WWR Scientific Products Co...	(800) 932-5000	1310 Goshen P...	West Chester
J. T. Baker	(800) 582-2537	222 Red School...	Phillipsburg
Promega Corp.	(800) 356-9526	2800 Woods Ho...	Madison
Pierce Chemical Co.	(800) 874-3723	3747 N Meridian...	Rockford
Mallinckrodt	(800) 354-2050	222 Red School...	Phillipsburg
ICN Pharmaceuticals, Inc.	(800) 854-0530	3300 Hyland Ave.	Costa Mesa
Bio-Rad Laboratories	(800) 424-6723	2000 Alfred Nob...	Hercules
Amersham Pharmacia Biote...	(800) 526-3593	800 Centennial ...	Piscataway
Invitrogen Corp.	(800) 955-6288	1600 Faraday A...	Carlsbad
Calbiochem-Novabiochem C...	(800) 854-3417	P.O. Box 12087	La Jolla
Hampton Research Corp.	(800) 452-3899	27632 El Lazo Rd.	Laguna Niguel

New... 18002

Update 18004

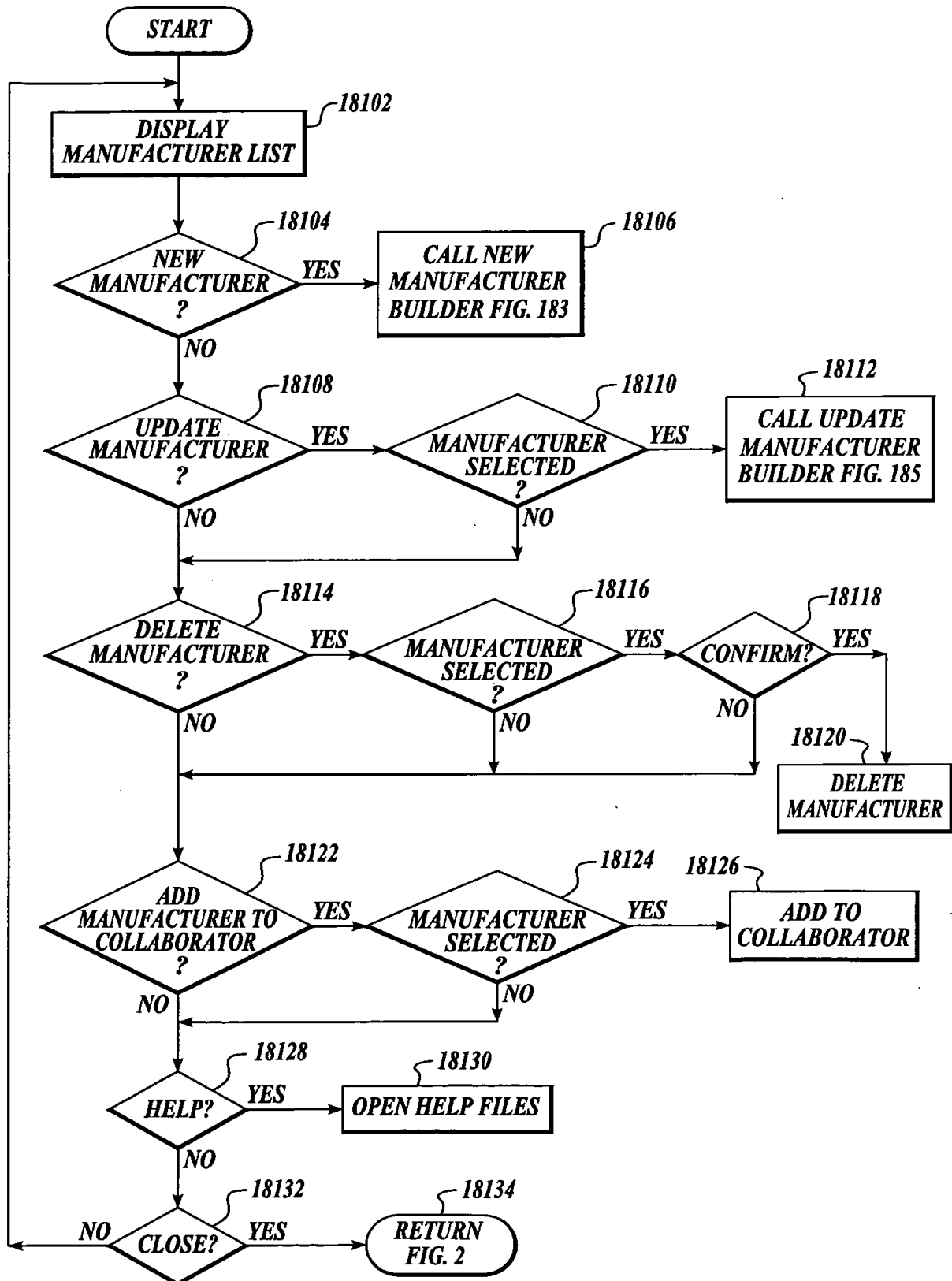
Delete 18006

Add to Collab 18008

Help... 18010

Close 18012

Fig. 180

*Fig. 181*

Update Emerald BioStructures, Inc. [X]

Name: 18200

Phone: 18202

Street: 18204

City: 18206

State: 18208

Zip: 18210

Country: 18212

Email: 18214

HTTP: 18216

Fax: 18218

Dept: 18220

18222

18224

18226

Fig. 182

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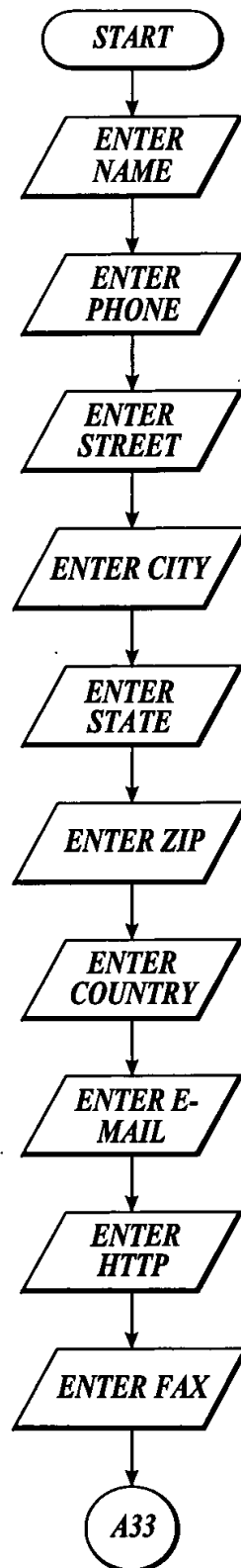
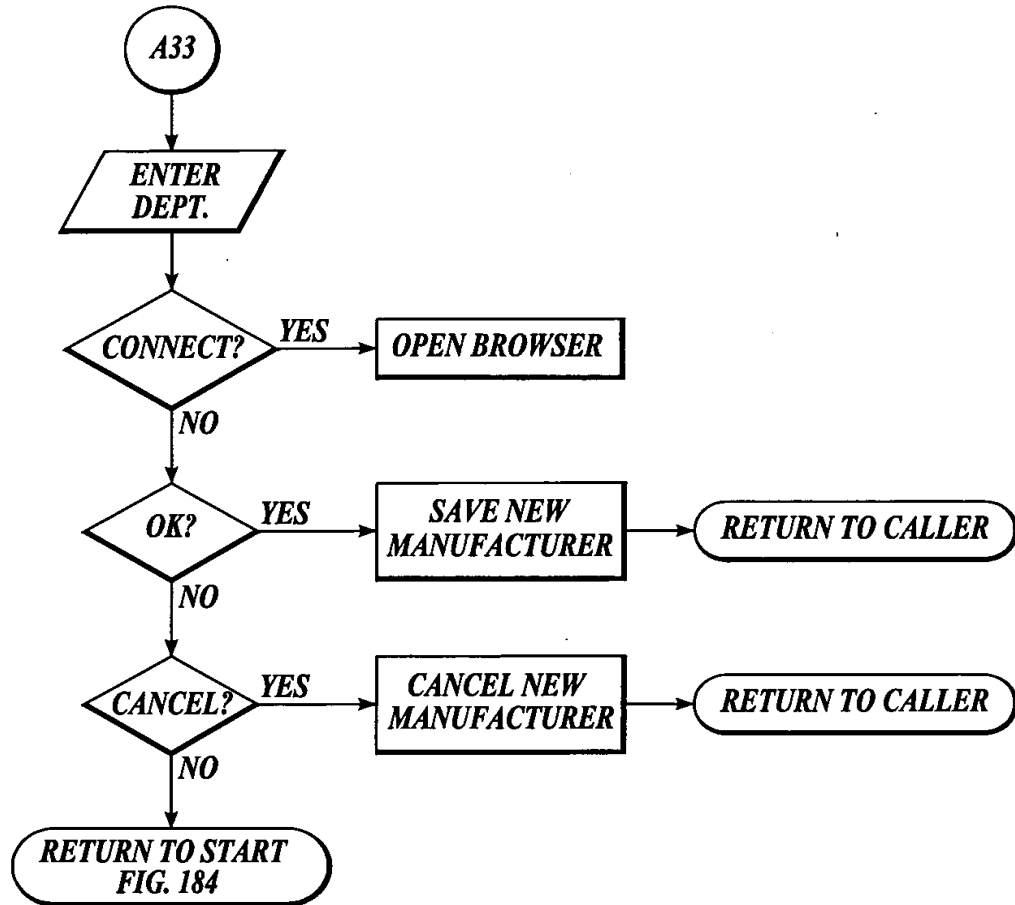


Fig. 183

*Fig. 184*

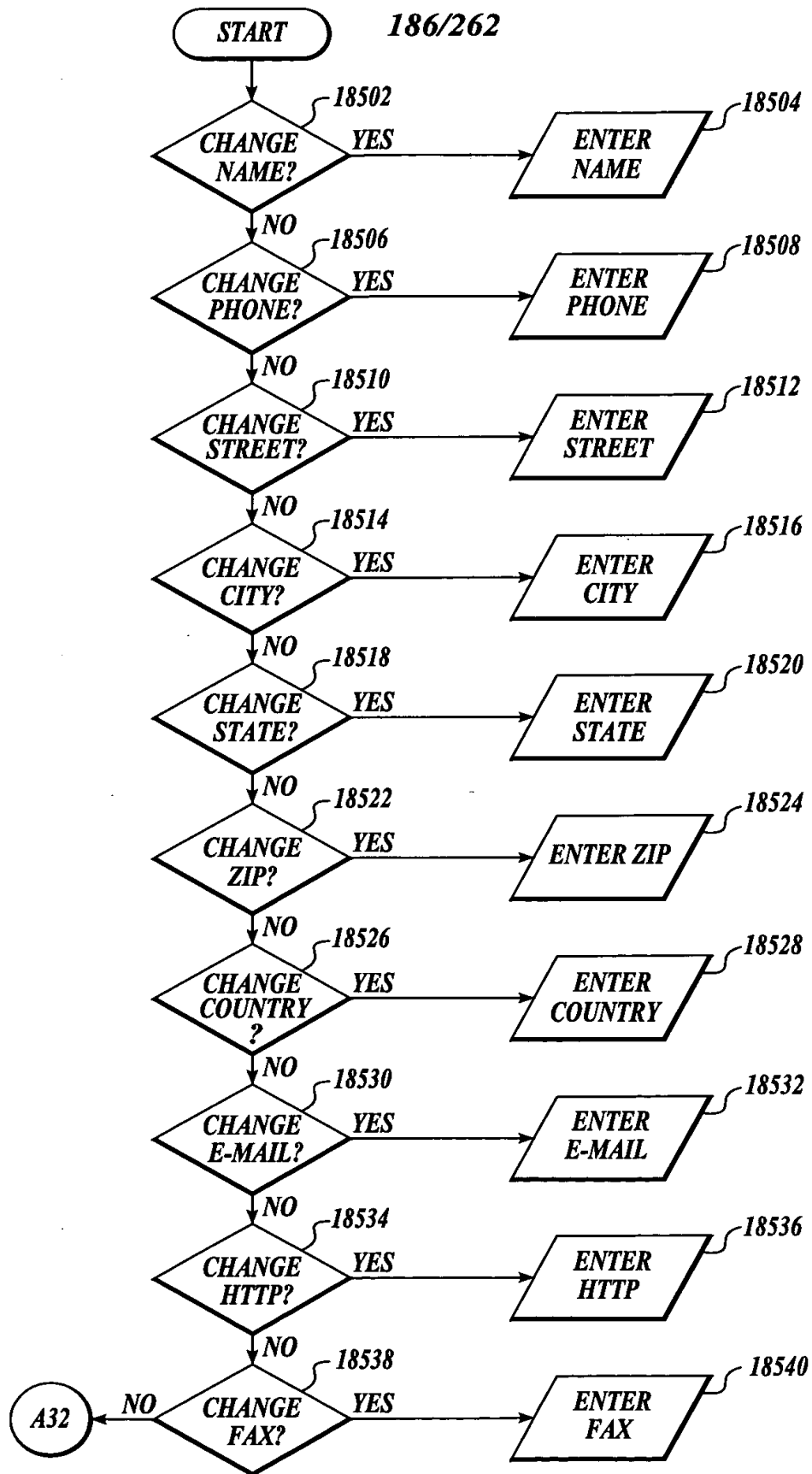
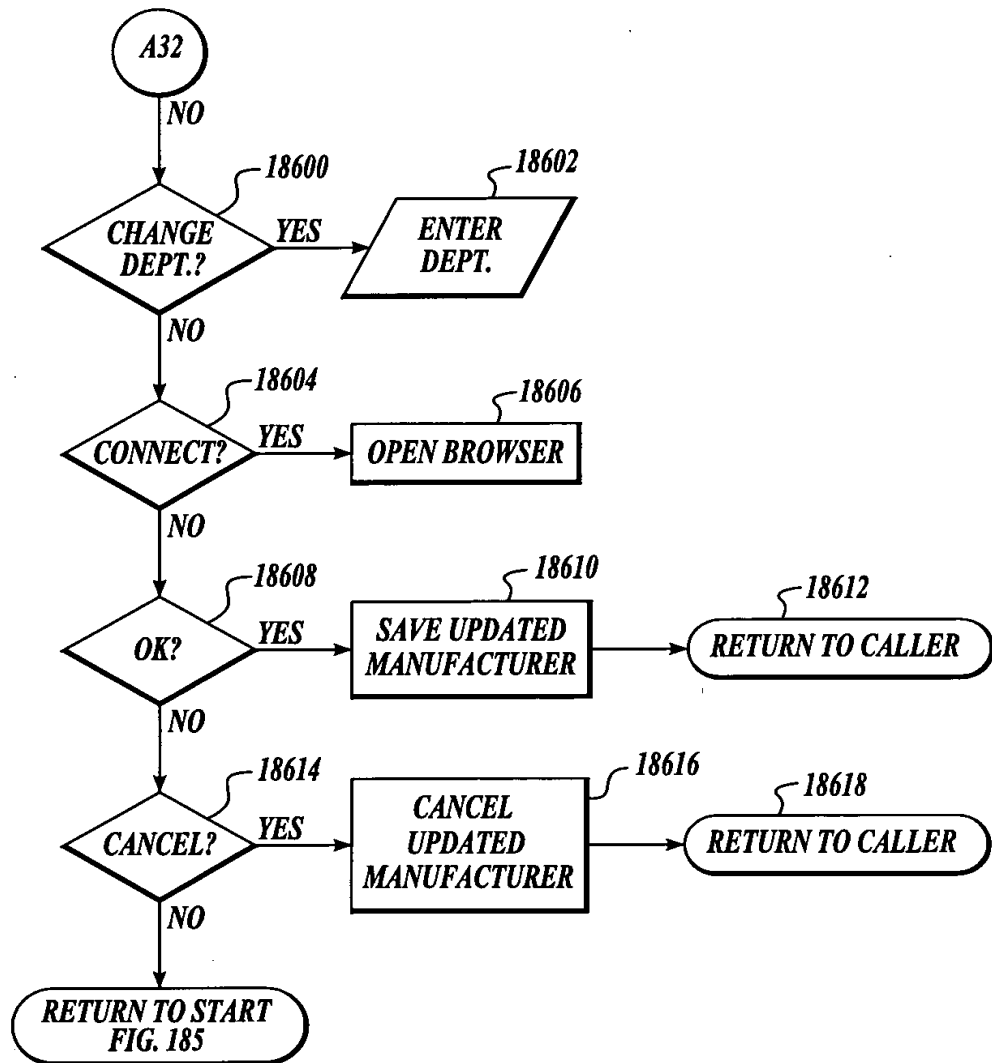
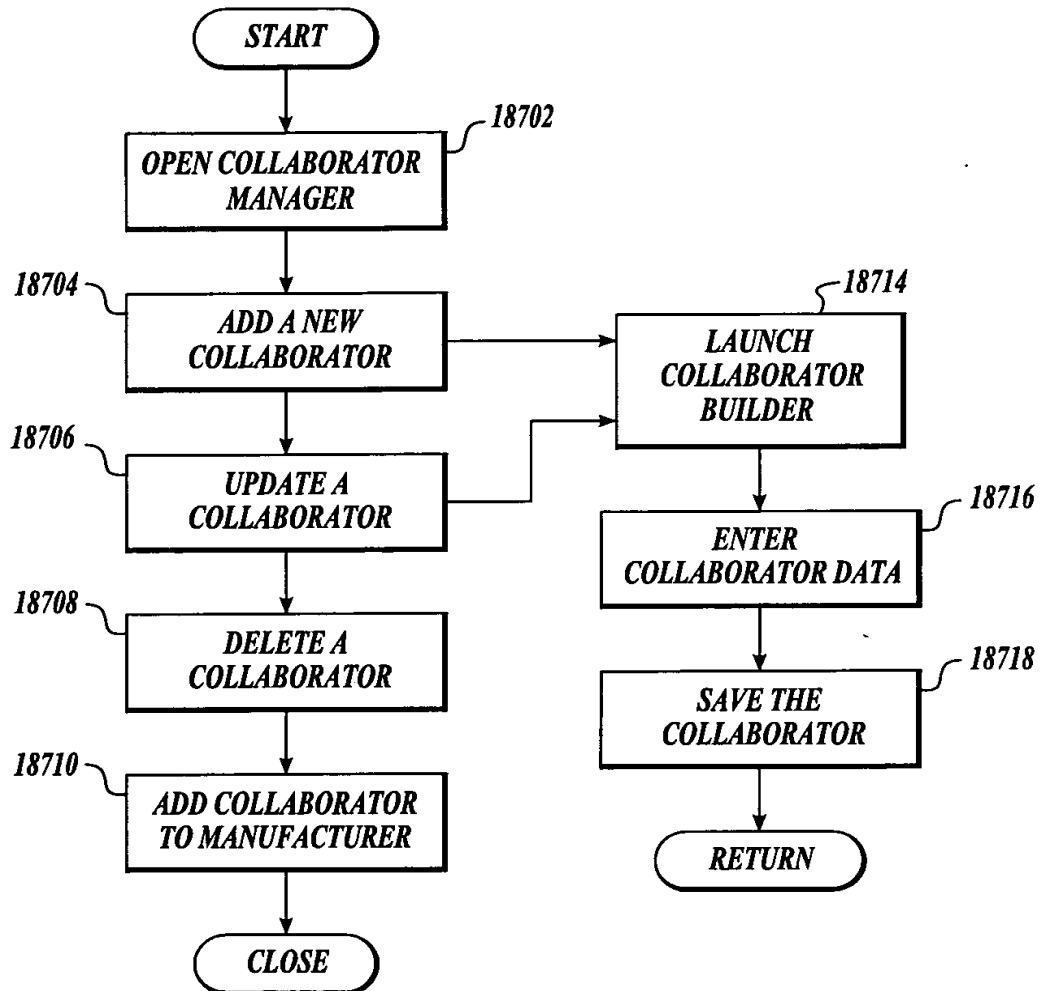
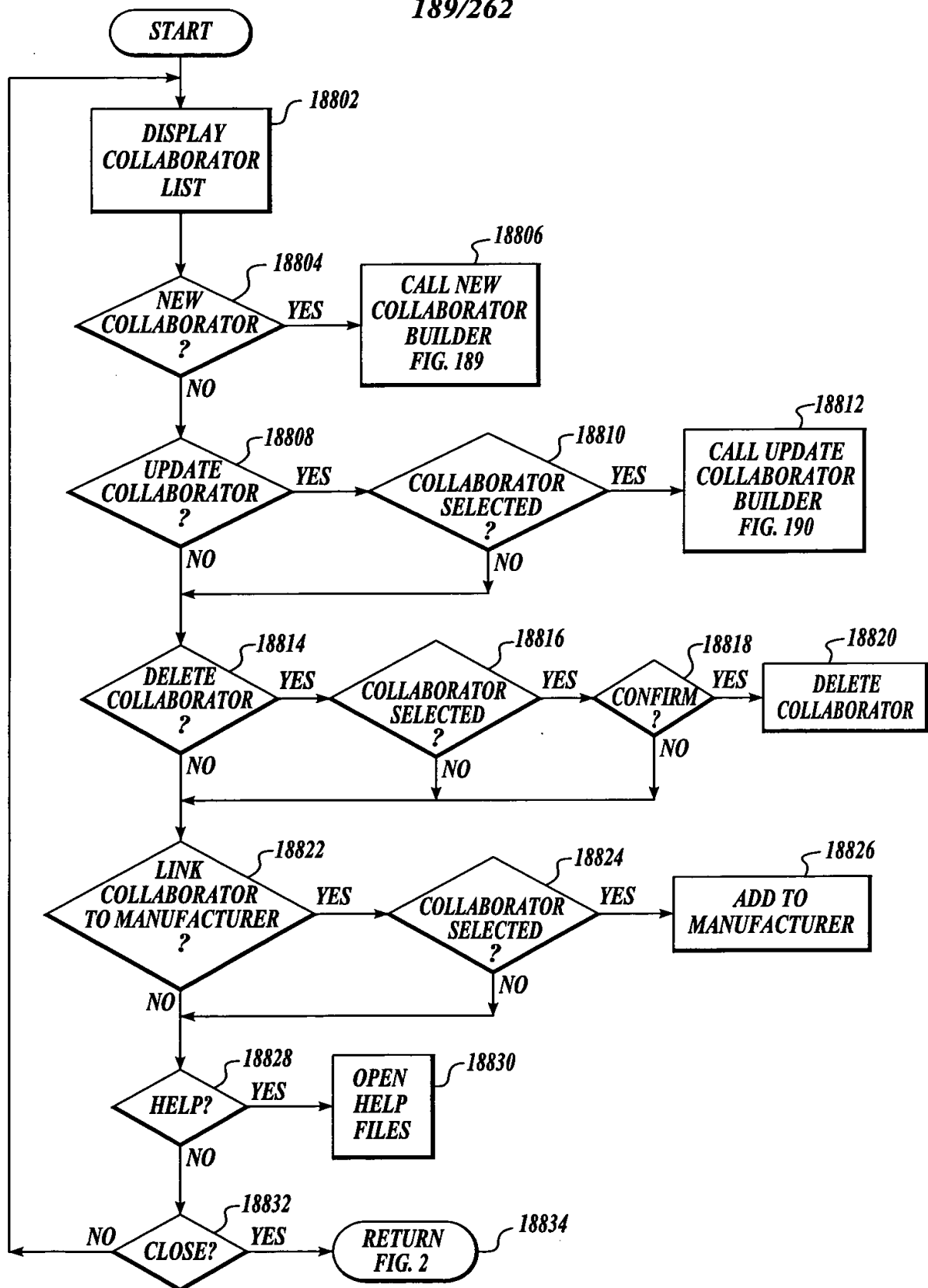


Fig. 185

*Fig. 186*

*Fig. 187*

*Fig. 188*

190/262

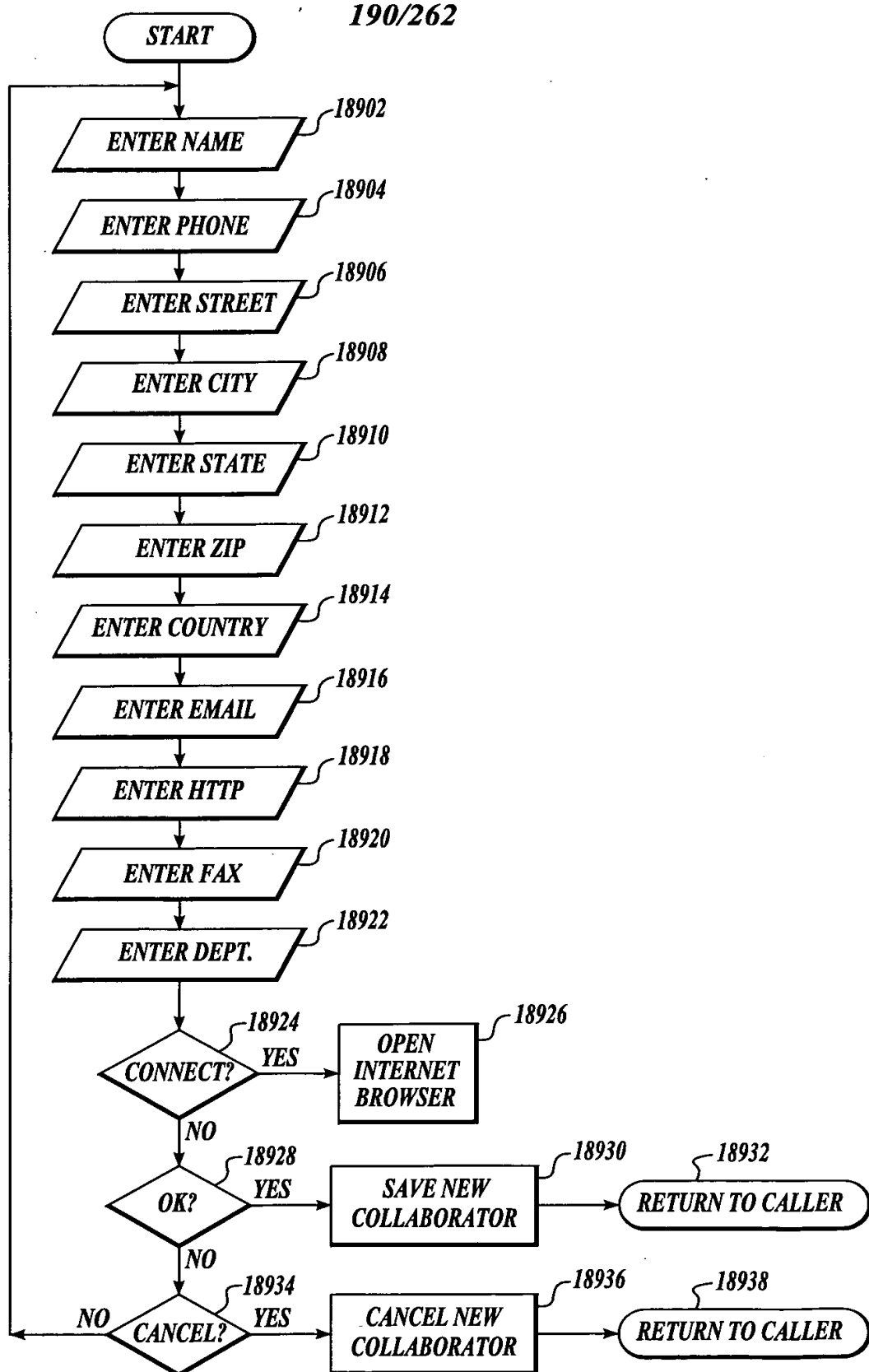
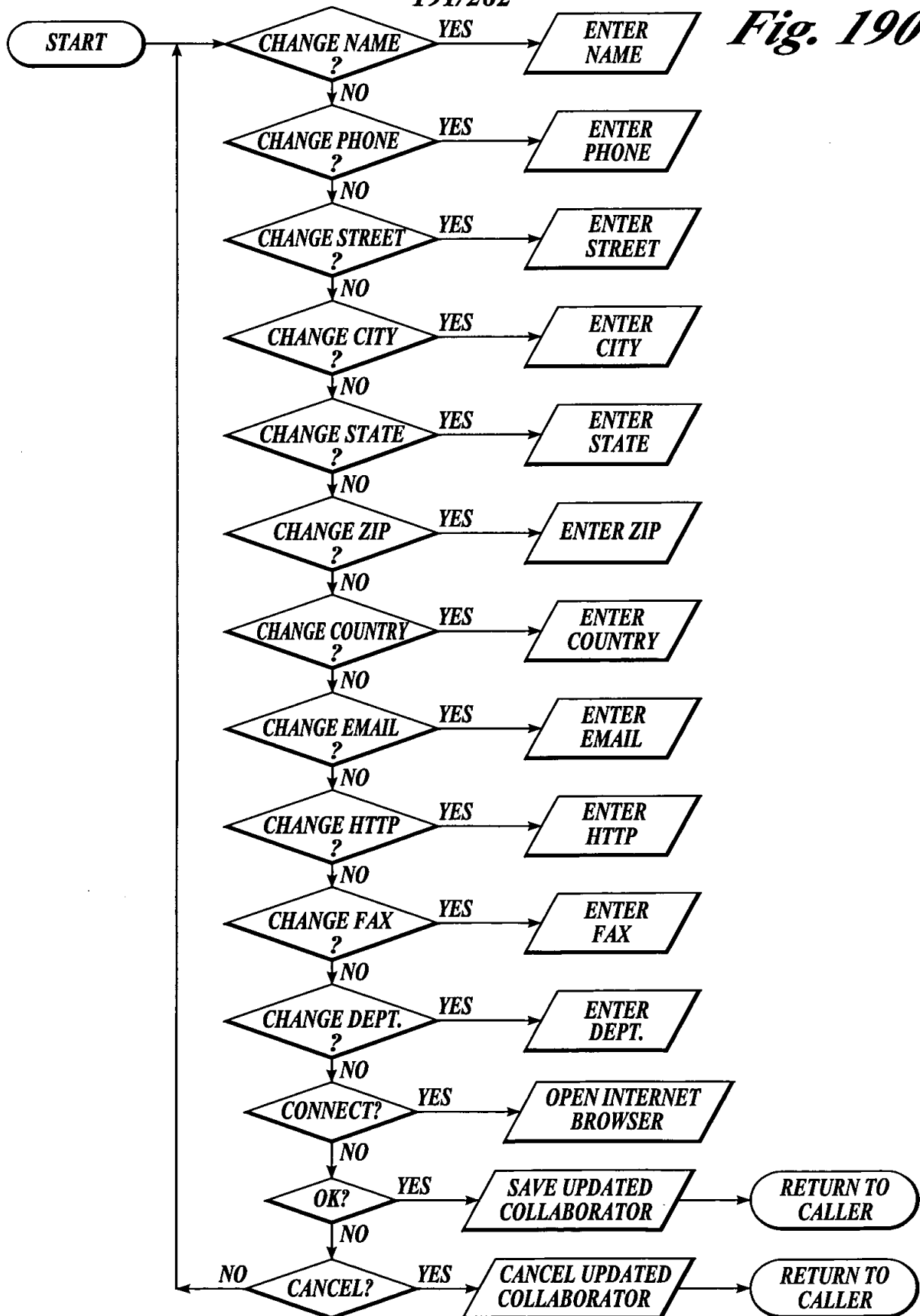
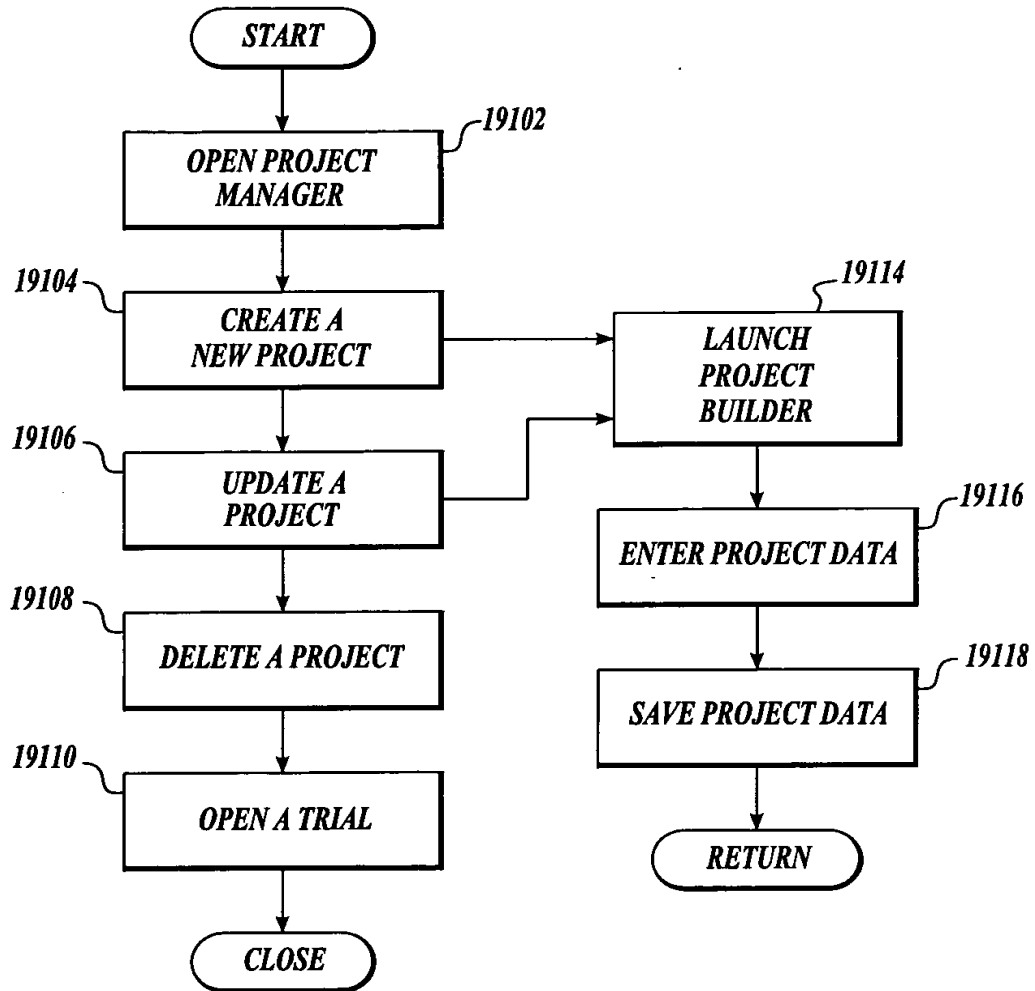


Fig. 189

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Fig. 190

*Fig. 191*

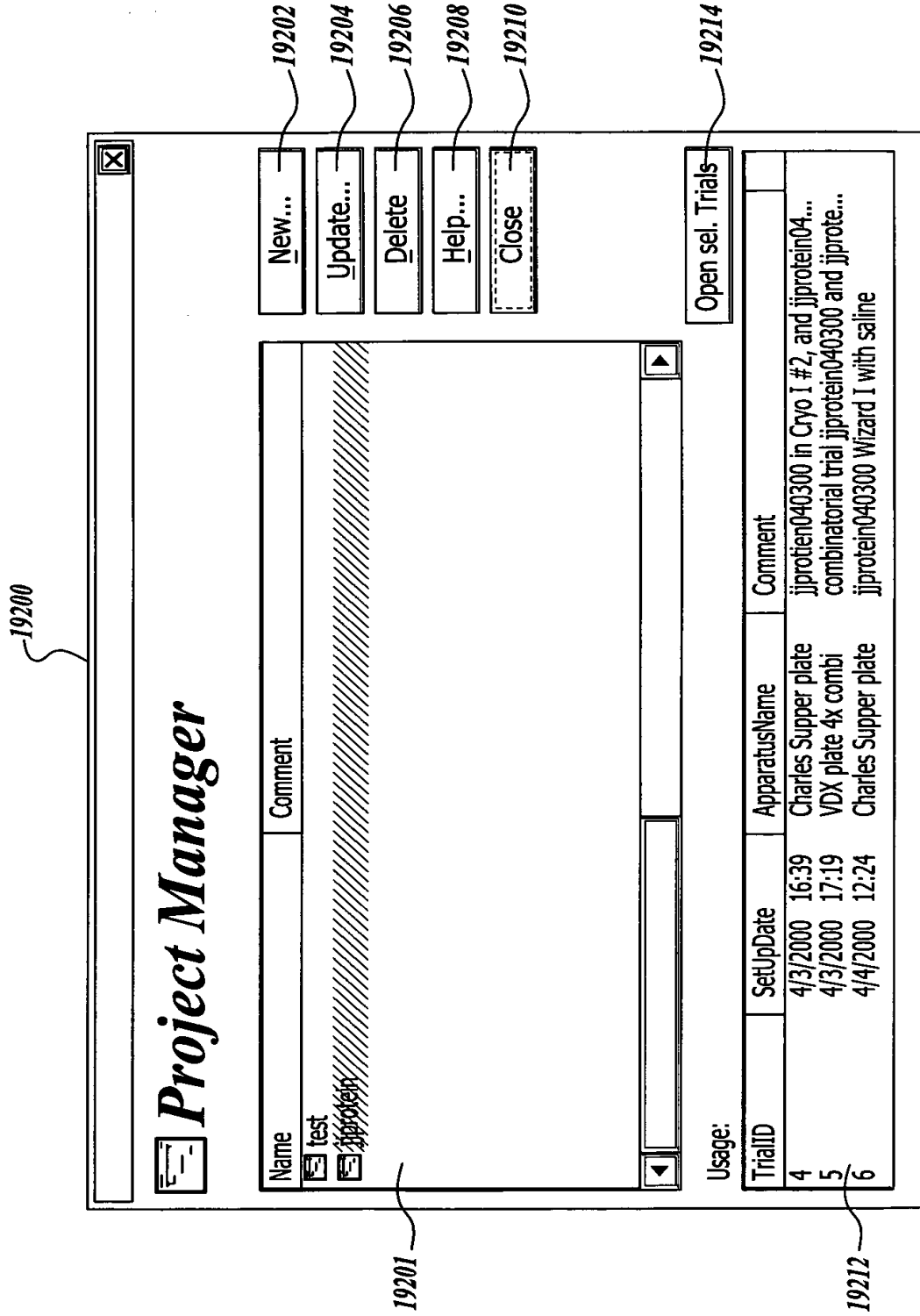
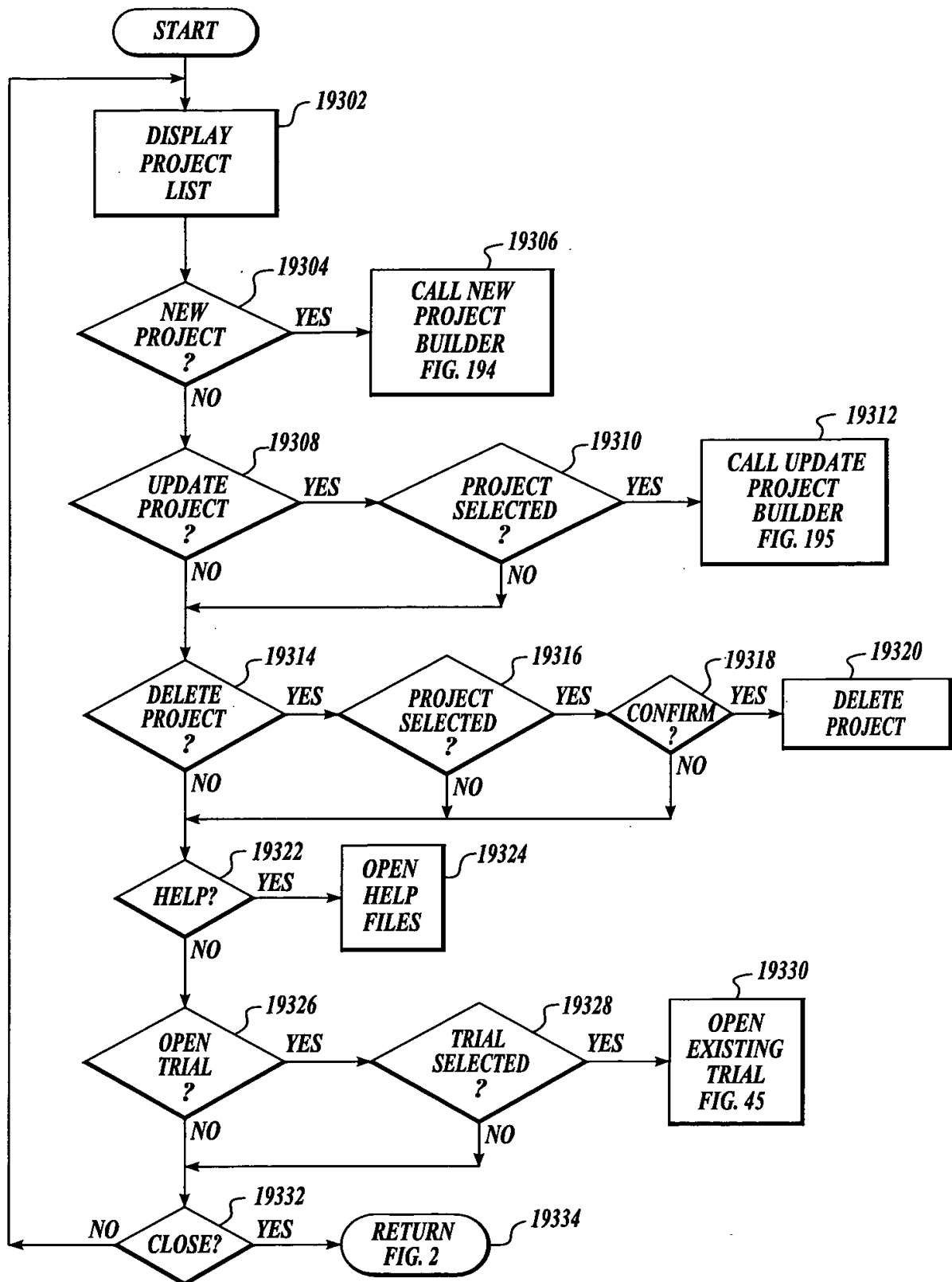
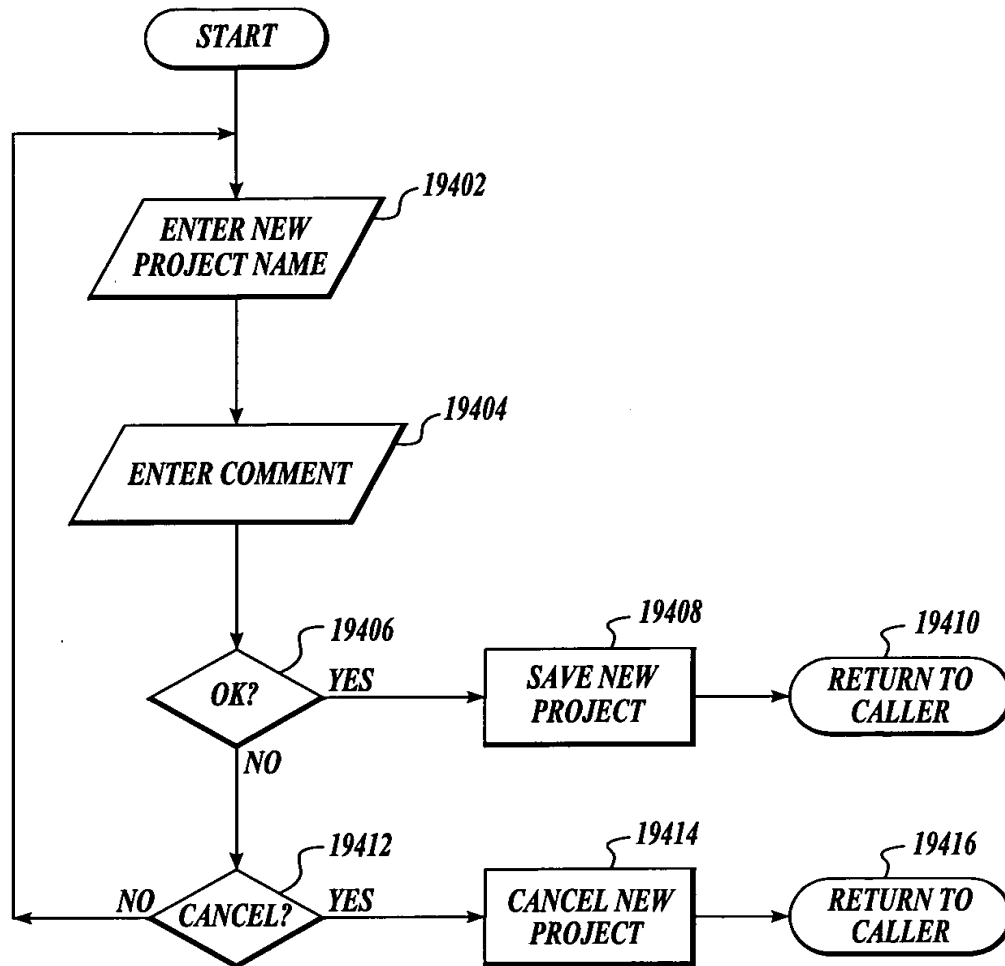
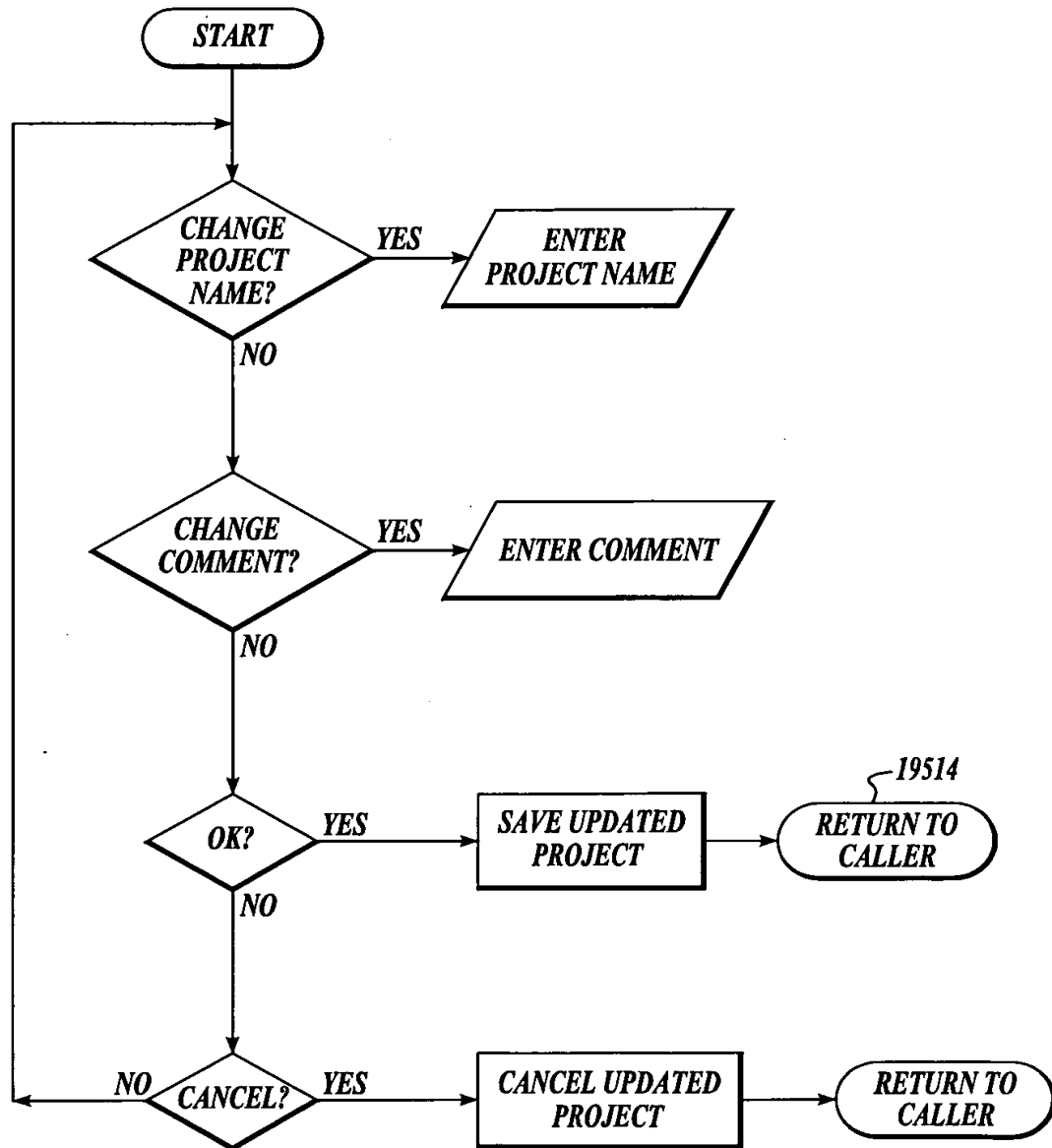
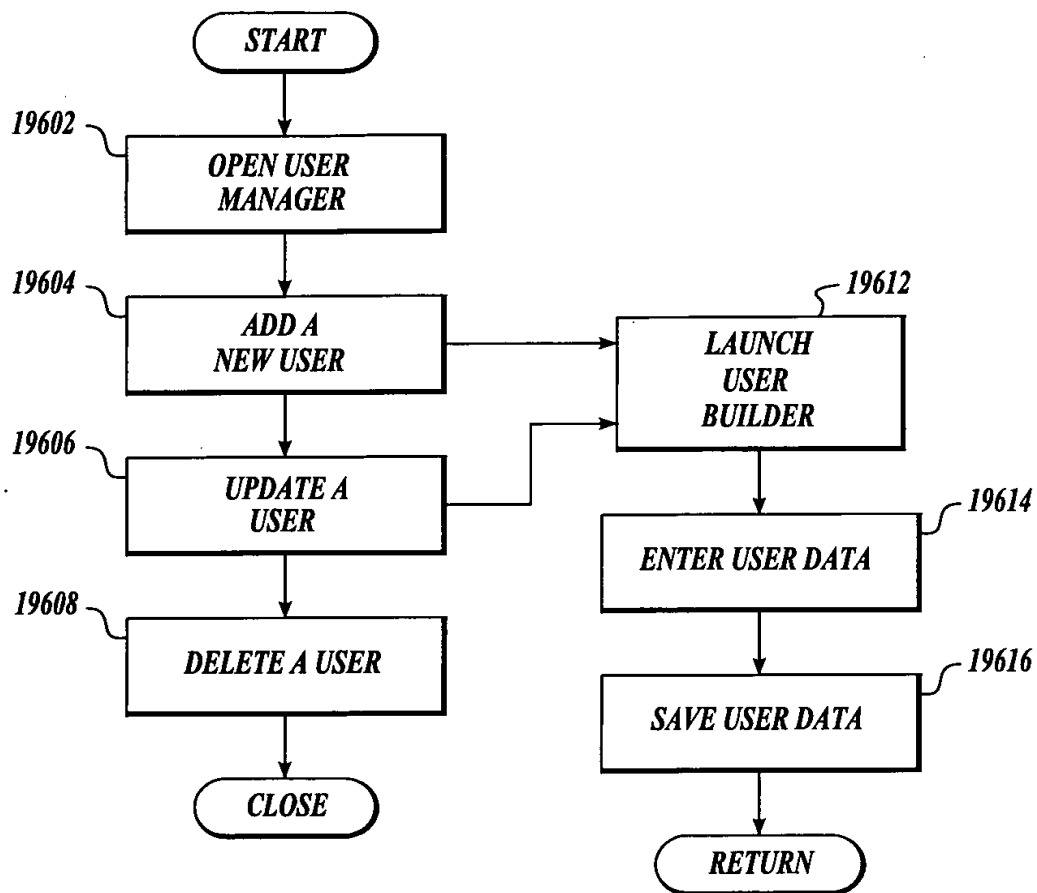


Fig. 192

*Fig. 193*

*Fig. 194*

*Fig. 195*

*Fig. 196*

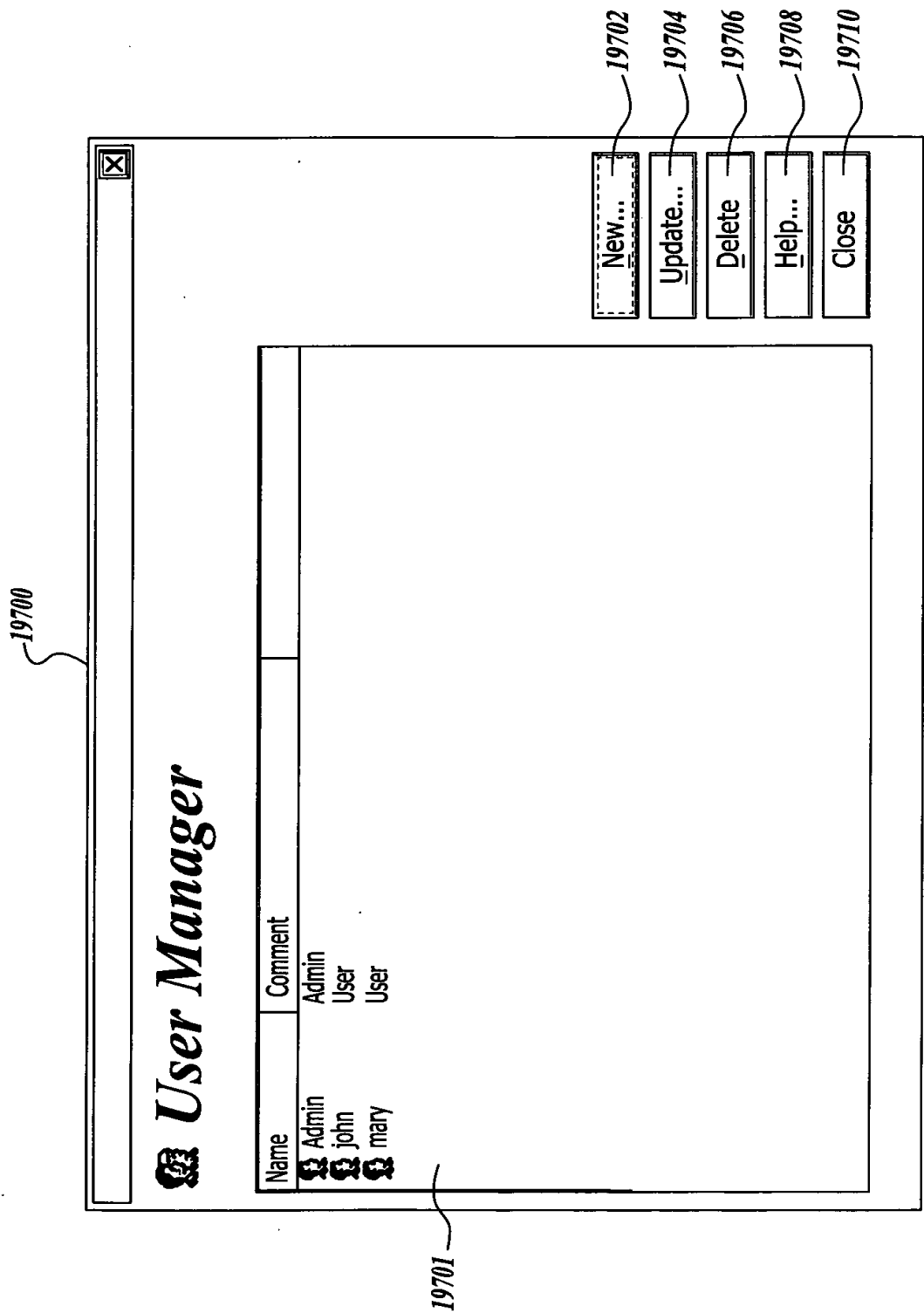
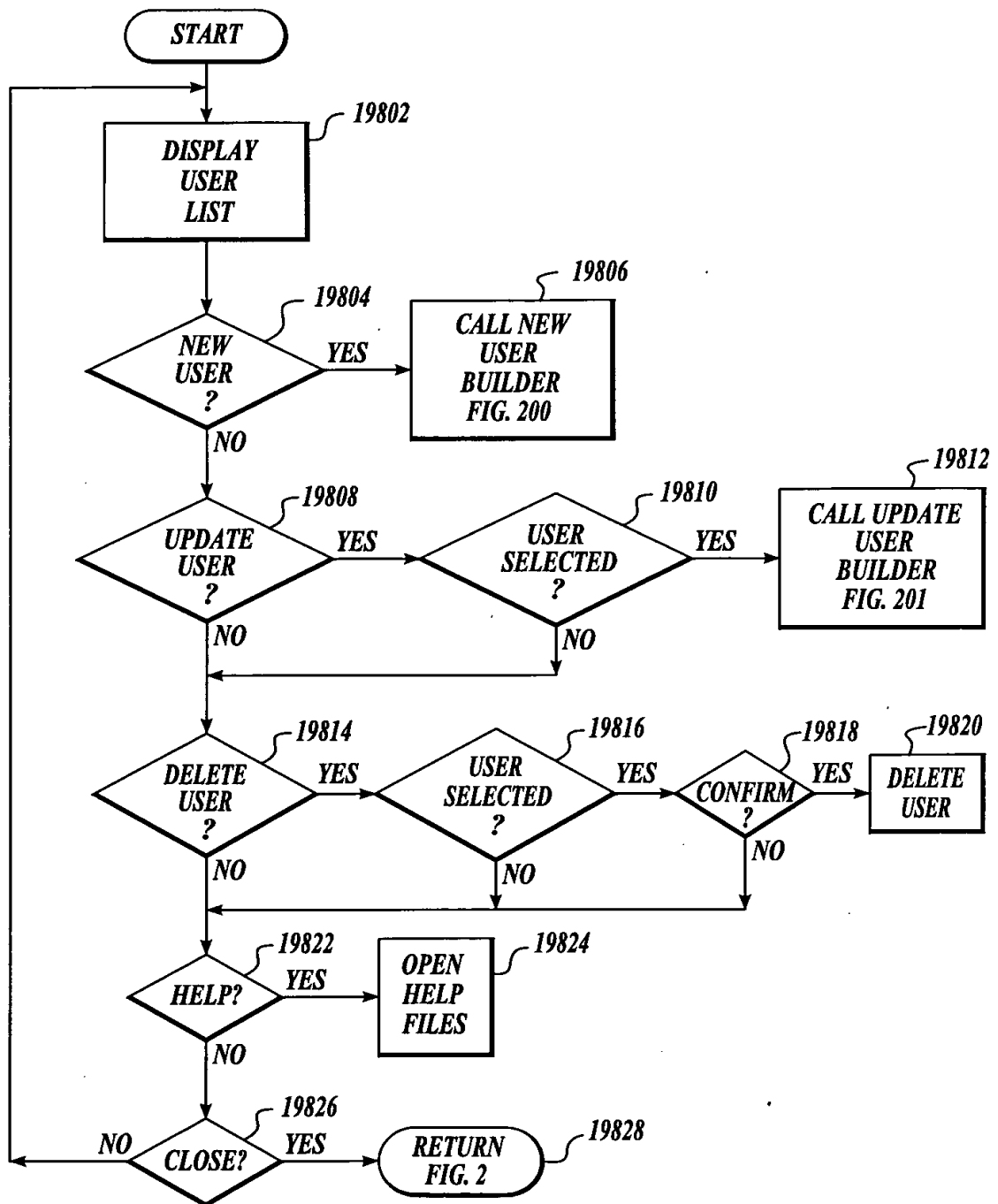
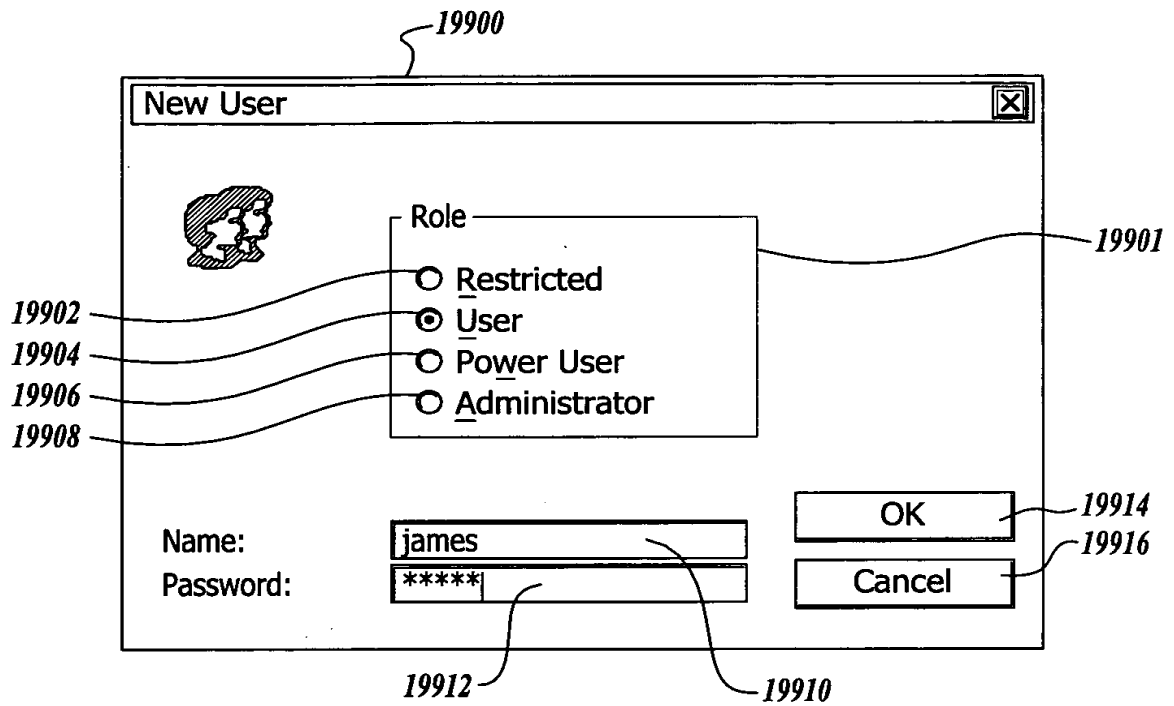
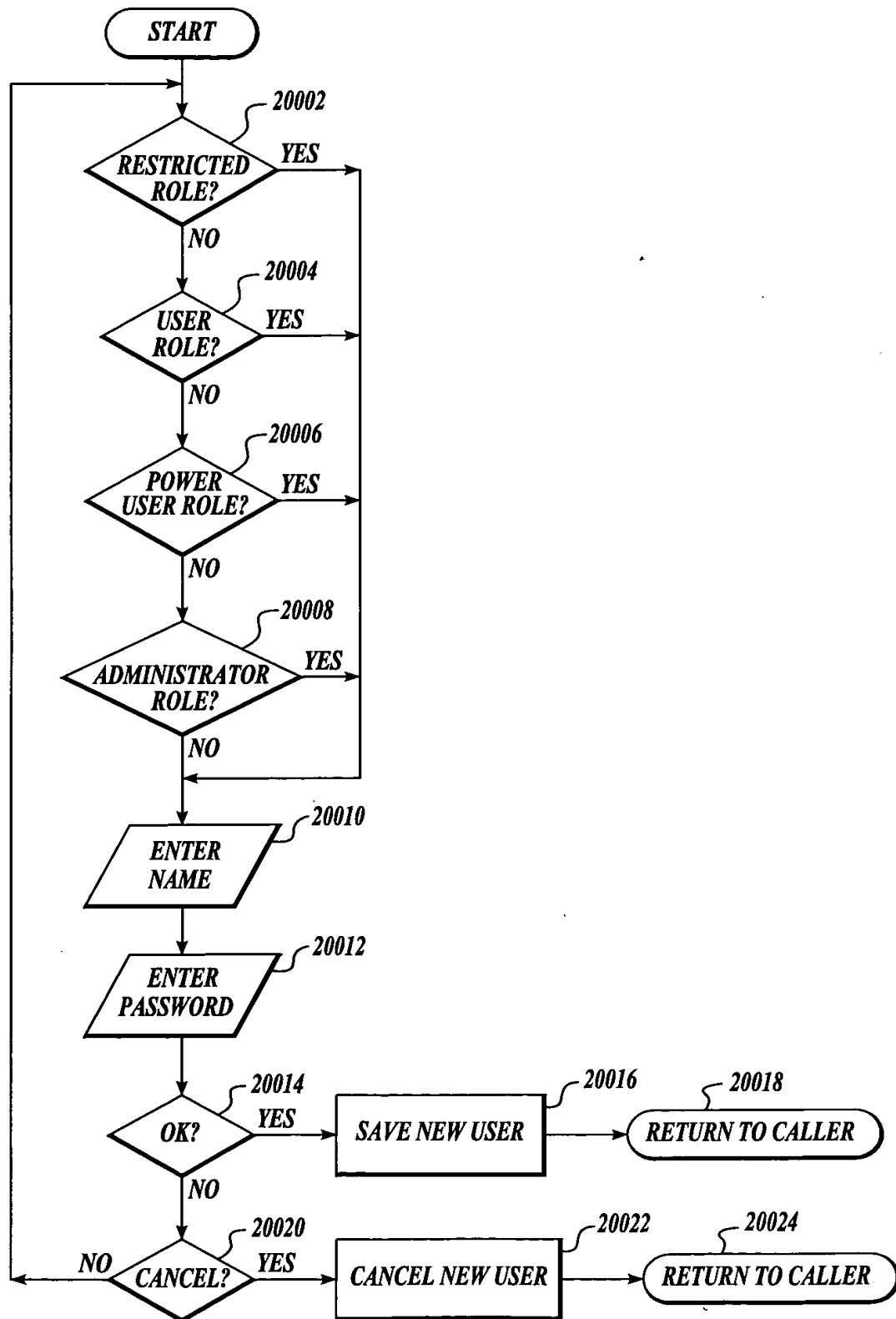
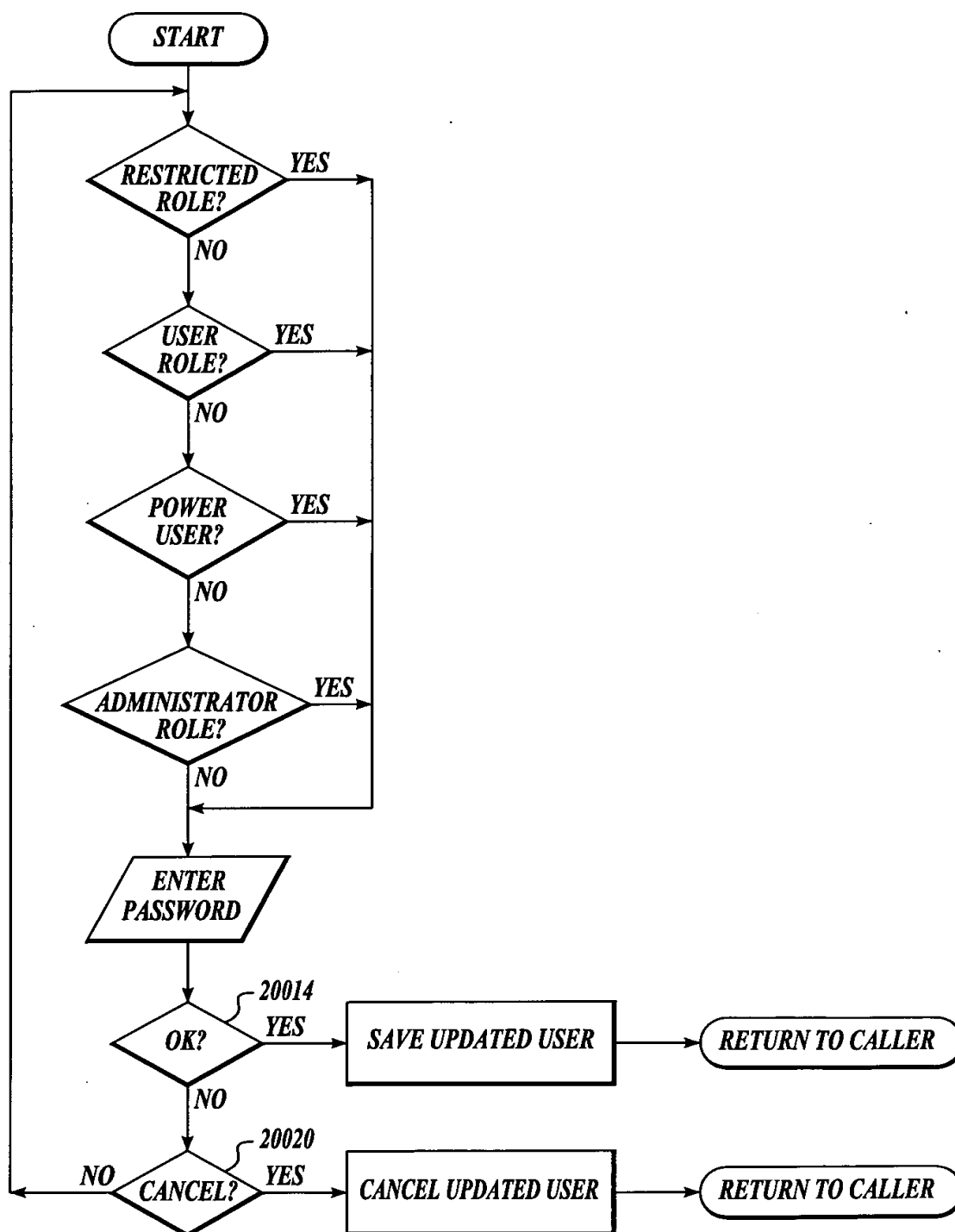


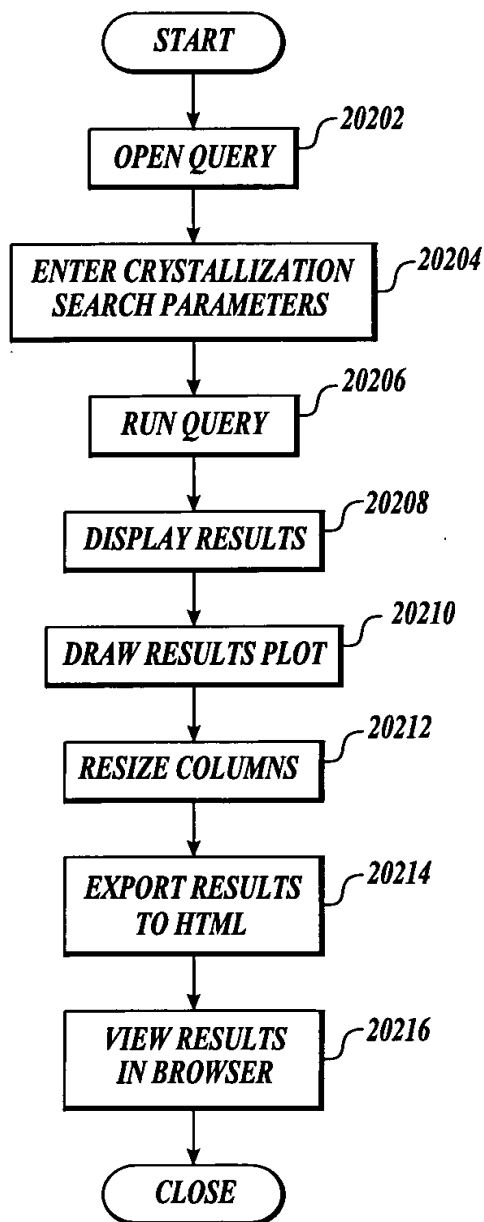
Fig. 197

*Fig. 198*

*Fig. 199*

*Fig. 200*

*Fig. 201*

*Fig. 202*

Crystal Query

Draw plot...

Query!

Fixed Resize

Exp. to HTML...

View in Browser...

20300

20301

20304

20306

20308

20310

20312

T...	S...	S./W.	Crystall...	Size	C...	Te...	Morphology	S	(Cplx-) Macro...	Compound Buffer
*** 3	3	07	Wzrd1 07	n/a	n/a	25.00	MicroCrystal		jjprotein040300	100.000 mM pH 6.00 MES/Na
• 3	3	13	Wzrd1 13	Tiny	1	25.00	Block		jjprotein040300	100.000 mM pH 6.50 Na cac
ε ³ 3	3	16	Wzrd1 16	Medium	n/a	25.00	Plate		jjprotein040300	100.000 mM pH 6.20 Na2 H p
▲ 3	3	17	Wzrd1 17	Small	5	25.00	Pyramid		jjprotein040300	100.000 mM pH 4.50 acetic a

Types

☐ Spherulite
☐ PhaseSep.
☐ Skin
☐ Precipitate
☒ MicroCrystal

Shapes

☒ Needle
☒ Plate
☒ Pyramid
☒ Block
☒ Hexagon
☒ Leaf
☒ Urchin
☒ Rod

Sizes

☒ Tiny
☒ Small
☒ Medium
☒ Big

Misc.

☐ Twin
☐ Clear
☐ Image

User def.

☐ Usr def 1
☐ Usr def 2
☐ Usr def 3

Help

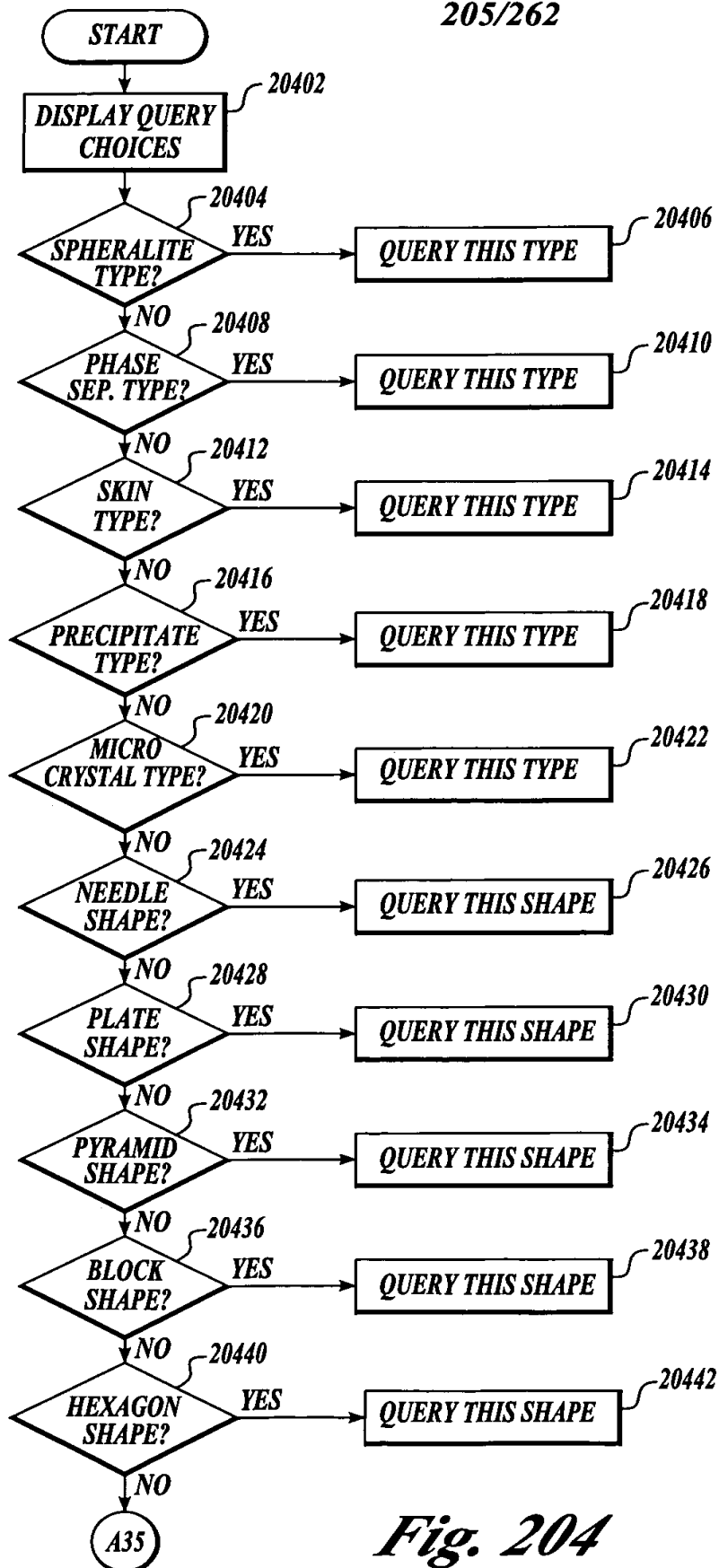
Close

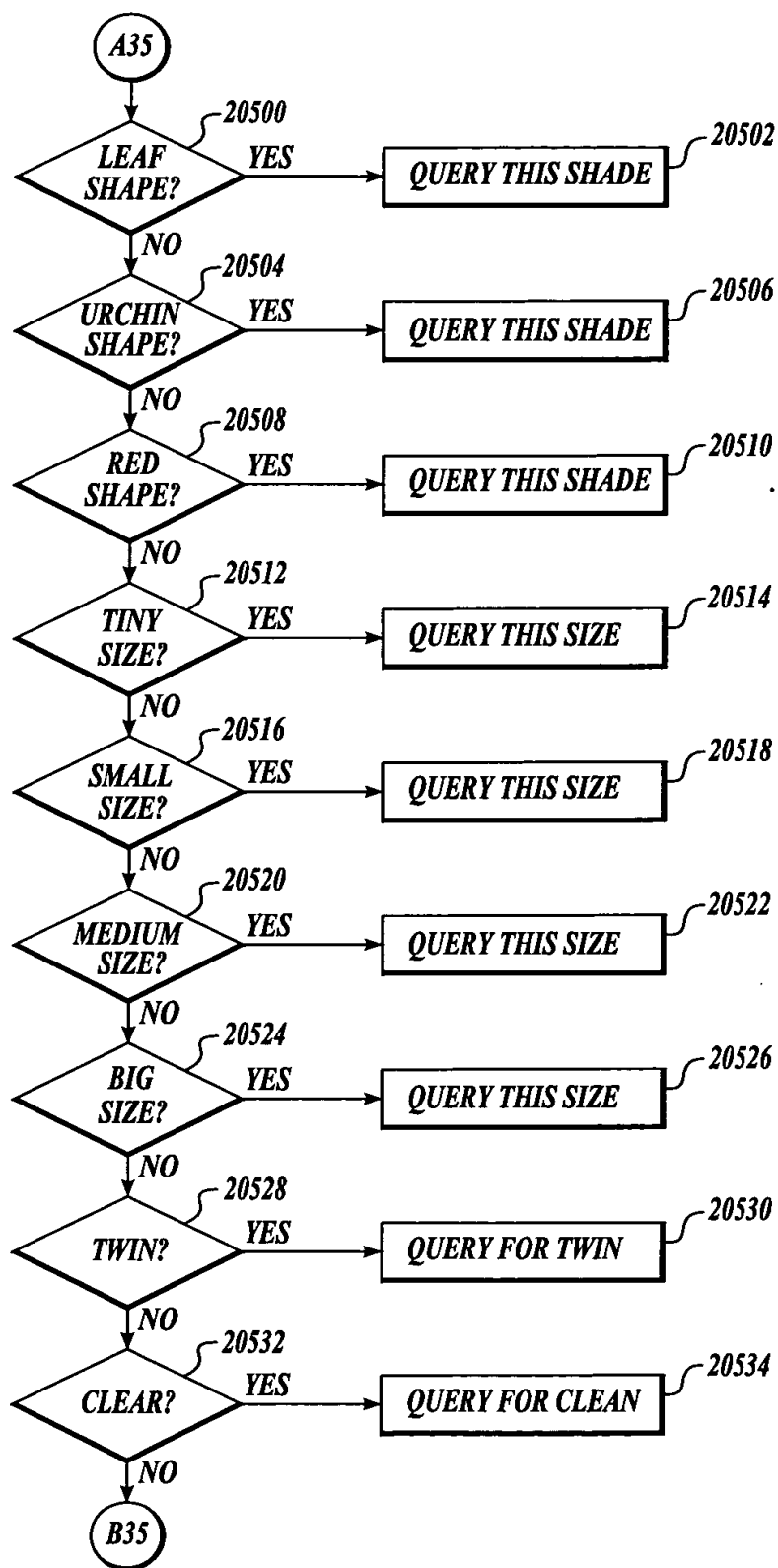
Help...

Observation sessions which are open and not in recording mode are queried. Click on column heading for sorting. Double-click on a row to see drop composition details.

204/262

Fig. 203

*Fig. 204*

*Fig. 205*

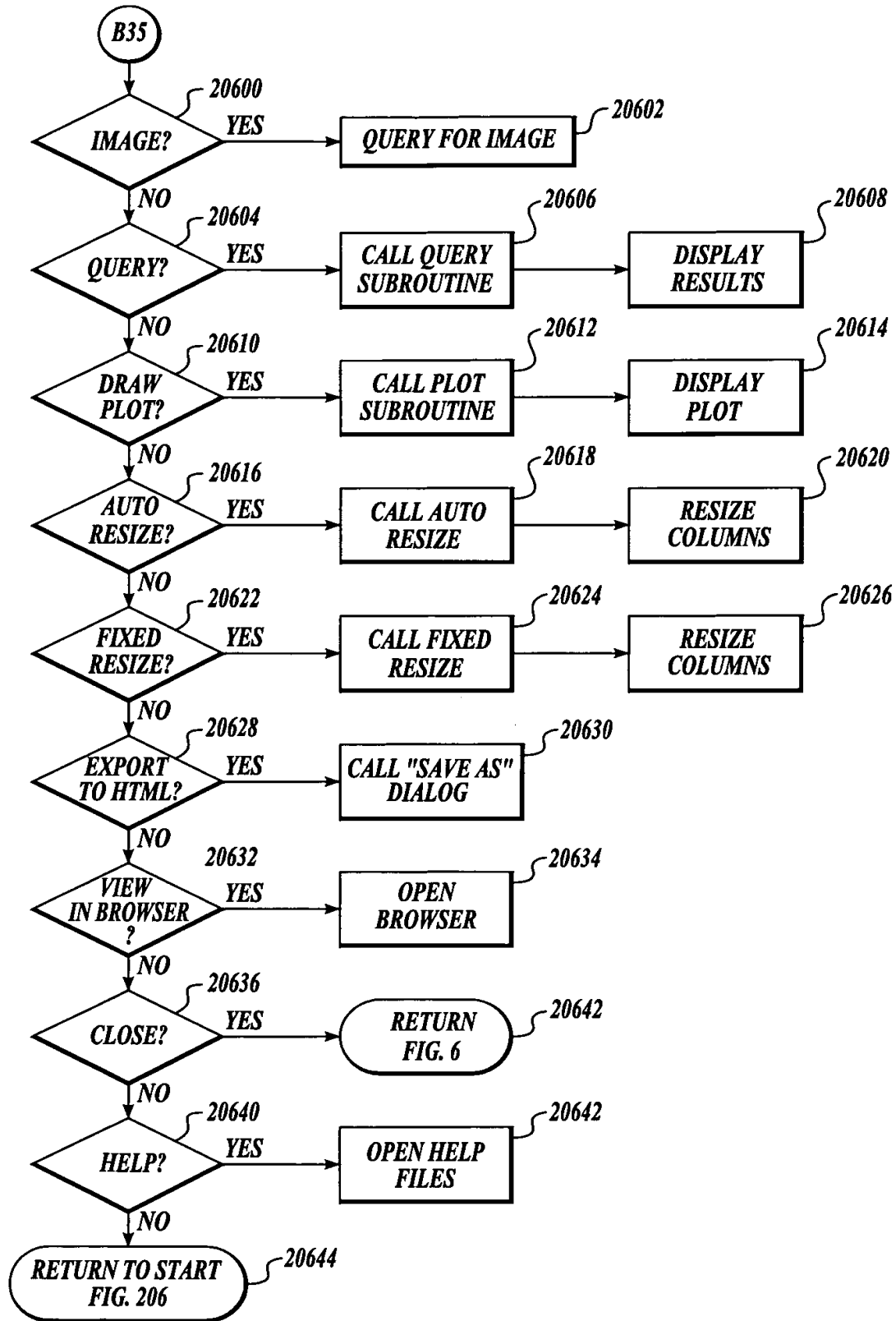


Fig. 206

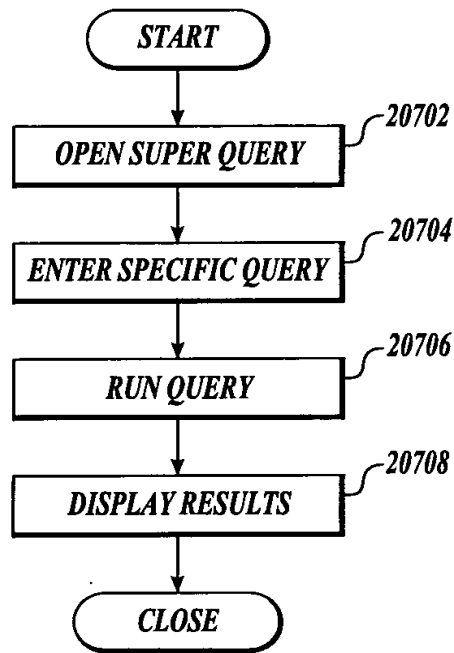


Fig. 207

20800

Crystal Monitor Super Query

Query #1: Show me all Trials where Crystals were obtained in the presence of the following chemical:

Catalog: CAS: Query:

20802 20804 20806

TrialID	SetUpDate	MatrixName	ProjectName	ApparatusName
3	4/3/2000 16:10	wzrd1	test	Charles Supper...

20801

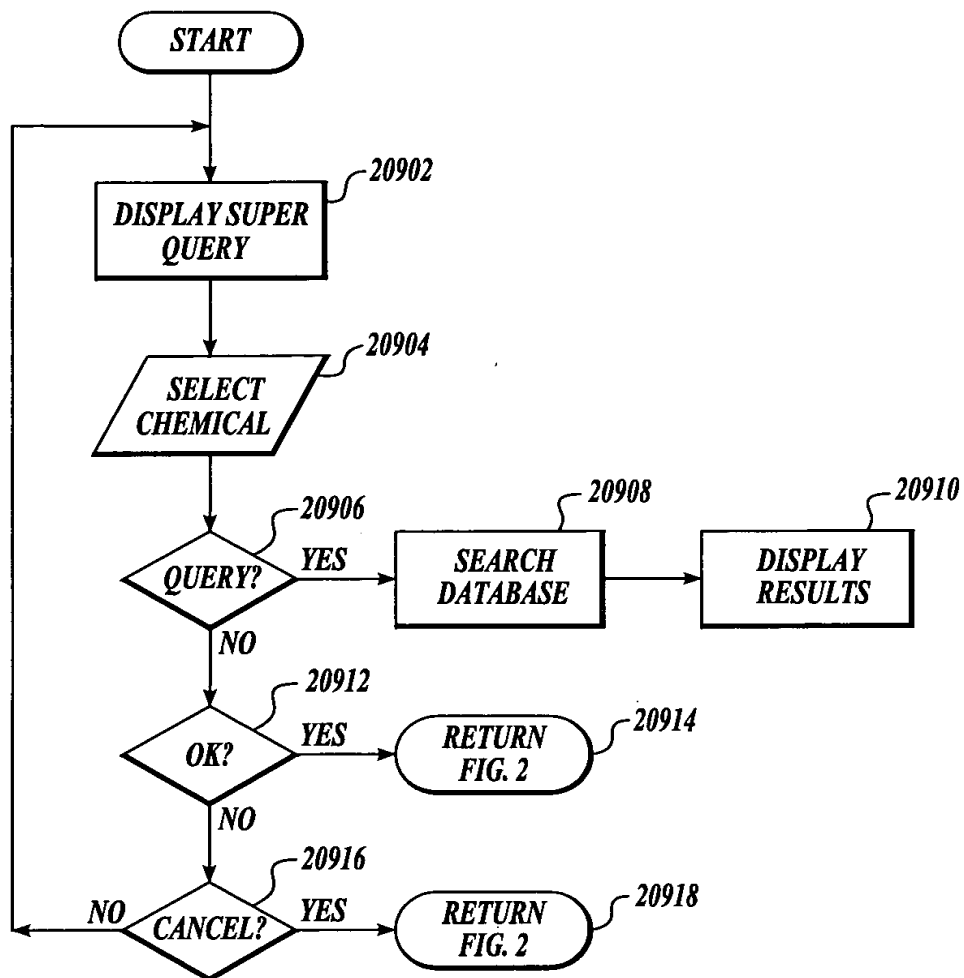
Notes

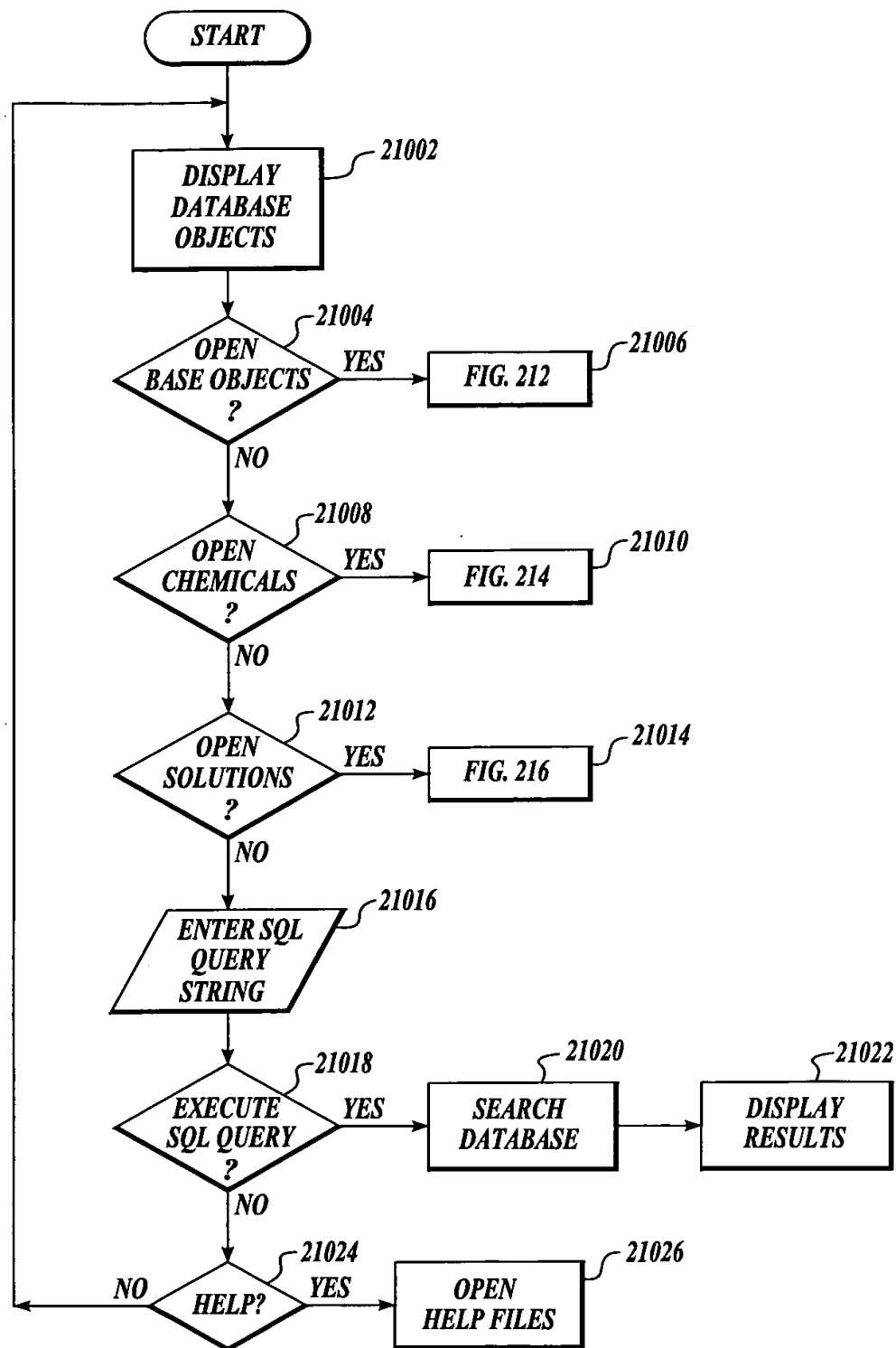
The super query is only a technology preview. Only one query is implemented. Many other queries will follow, once enough feedback has been collected from customers. Please send any query request to support@emeraldbiostructures.com.

OK Cancel Help...

20808 20810 20812

Fig. 208

*Fig. 209*

*Fig. 210*

21100

Database Object Manager

Crystal Monitor Objects:

- Base Objects
- Chemicals
 - Buffering Agent
 - pHConjugate
 - Precipitant
 - Salt
 - CSI
 - Chelator
 - Detergent
 - ReducingAgent
 - CryoCoolant
 - NucleationSuppressant
 - Organic
 - heavyAtomCompound
 - Metal
 - Gas
 - Solvent
 - Other
- Solutions
- Data Mining

Attributes:

ChemicalName	ShortName	Formula	MolecularMass
dimethylarsinic...	sodium cacodyl...	C ₂ H ₆ AsO ₂ Na	160.
sodium citrate tri...	sodium citrate	C ₆ H ₅ Na ₃ O ₇ *2H...	294.1
ammonium sulfate	ammonium sulfate	(NH ₄) ₂ SO ₄	132.1
ammonium sulfate	ammonium sulfate	(NH ₄) ₂ SO ₄	132.1
ammonium sulfate	ammonium sulfate	(NH ₄) ₂ SO ₄	132.1
lithium sulfate m...	lithium sulfate	Li ₂ SO ₄ *H ₂ O	128.
ammonium phos...	dibasic ammoniu...	(NH ₄) ₂ HPO ₄	132.1
sodium chloride	sodium chloride	NaCl	58.44
sodium phospha...	monobasic sodi...	NaH ₂ PO ₄	120.
sodium phospha...	monobasic sodi...	NaH ₂ PO ₄	120.
sodium phospha...	monobasic sodi...	NaH ₂ PO ₄	119.96
potassium sodiu...	K/Na tartrate	C ₄ H ₄ O ₆ NaK*4H...	282.2
sodium formate	sodium formate	CHO ₂ Na	68.01
zinc acetate di...	zinc acetate	Zn(C ₂ H ₃ O ₂) ₂ *2...	219.5
magnesium chlo...	magnesium chlo...	MgCl ₂ *6H ₂ O	203.3
calcium acetate	calcium acetate	Ca(C ₂ H ₃ O ₂) ₂	158.2
magnesium acet...	magnesium acet...	Mg(C ₂ H ₃ O ₂) ₂ *4...	214.5

Execute SQL Query

26 rows. Query time:411ms

Help...

Fig. 211

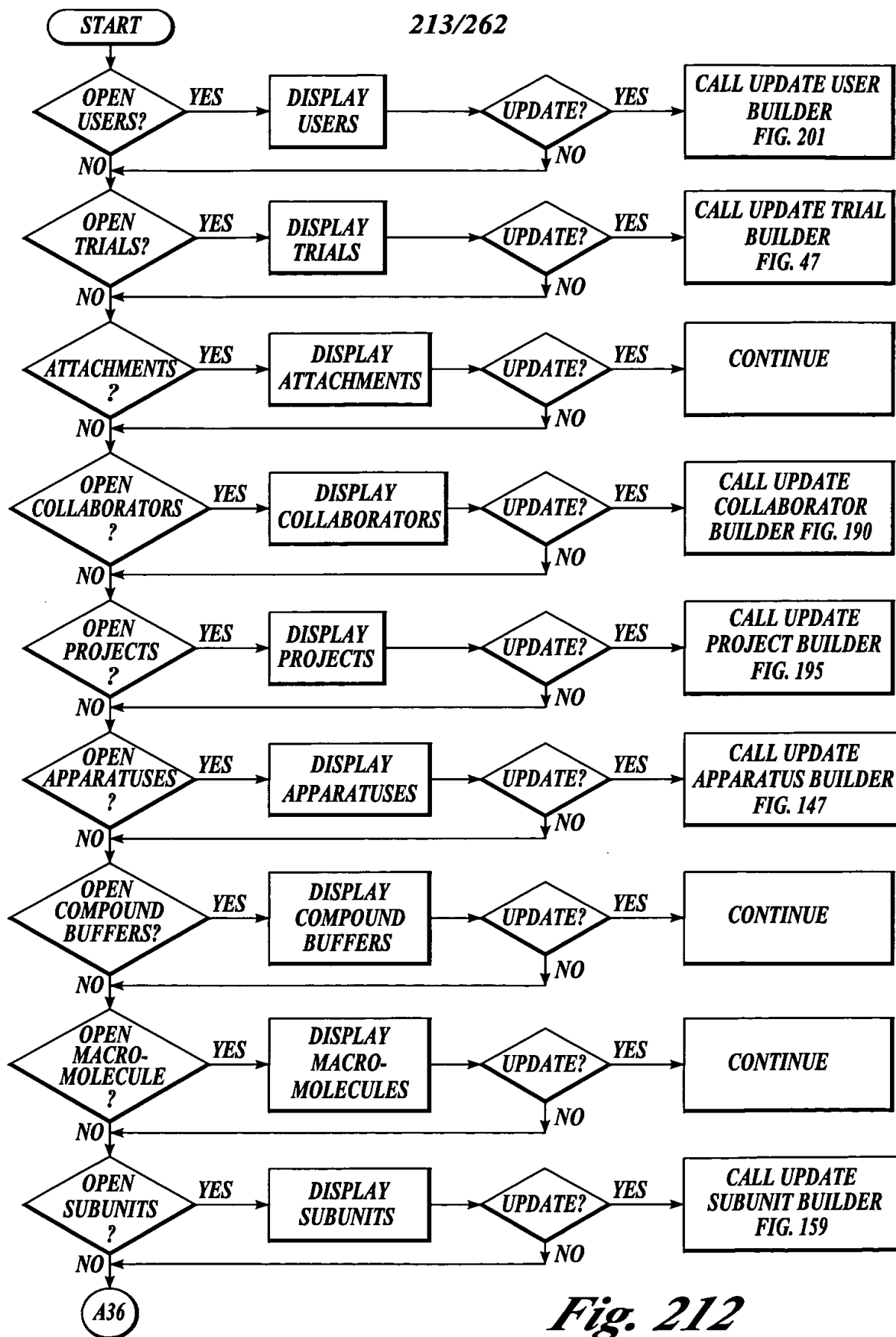
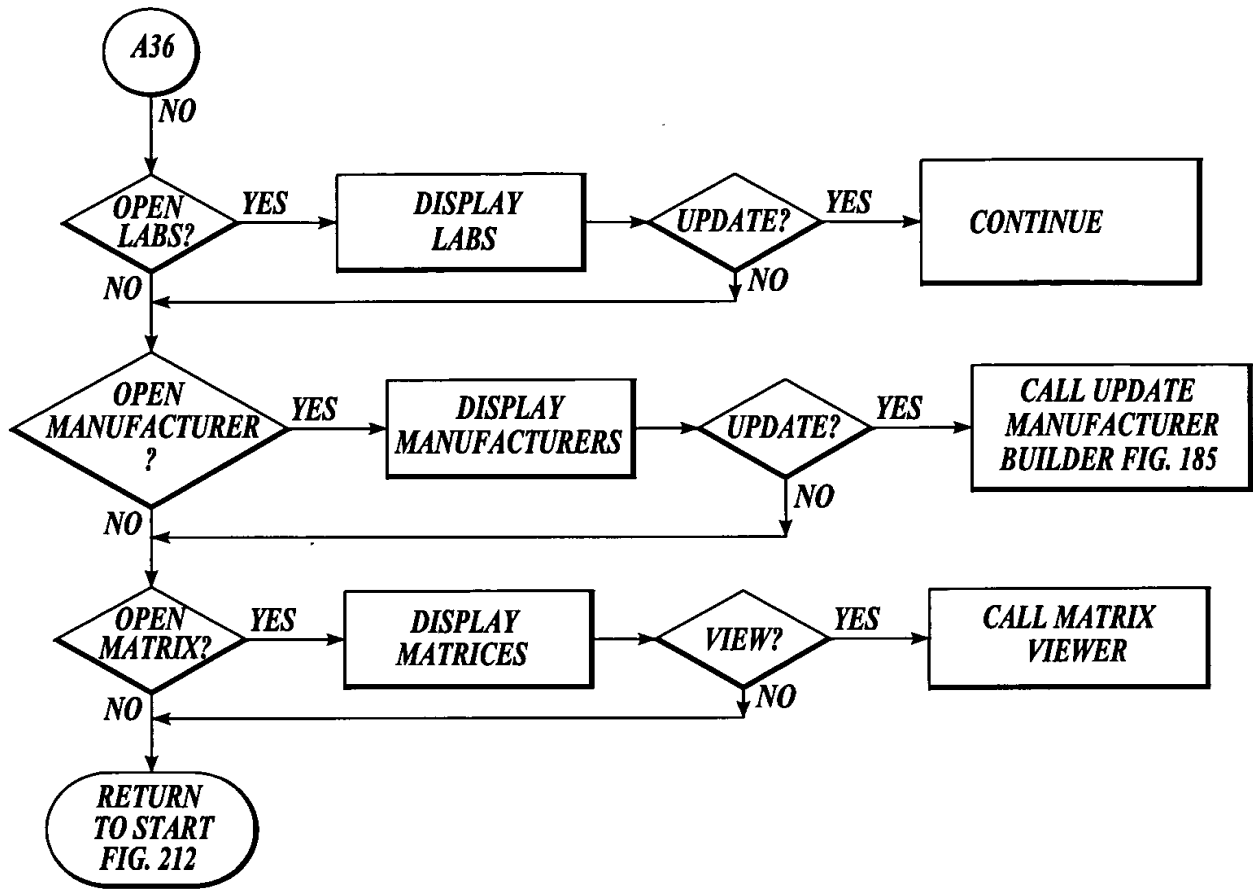
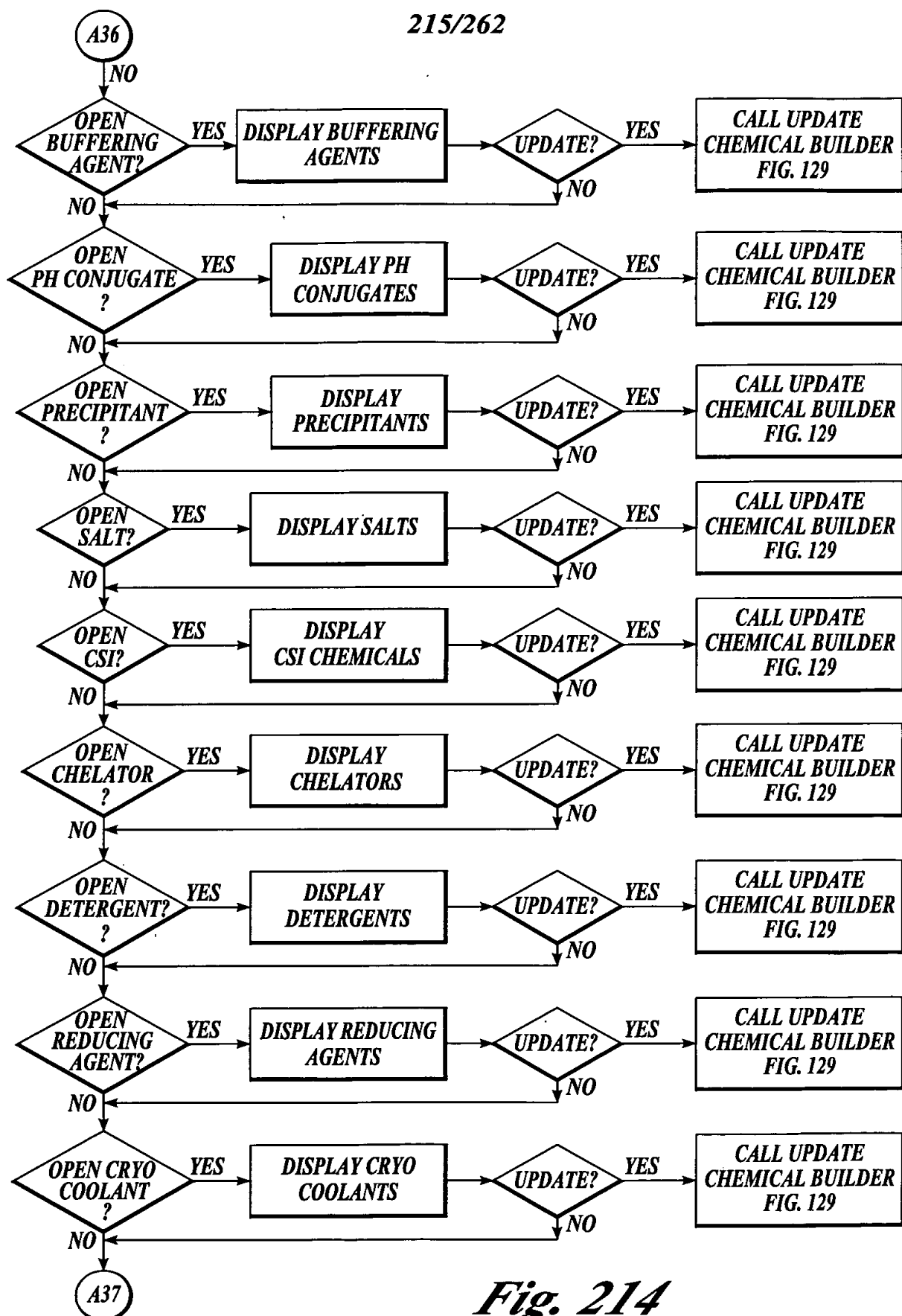
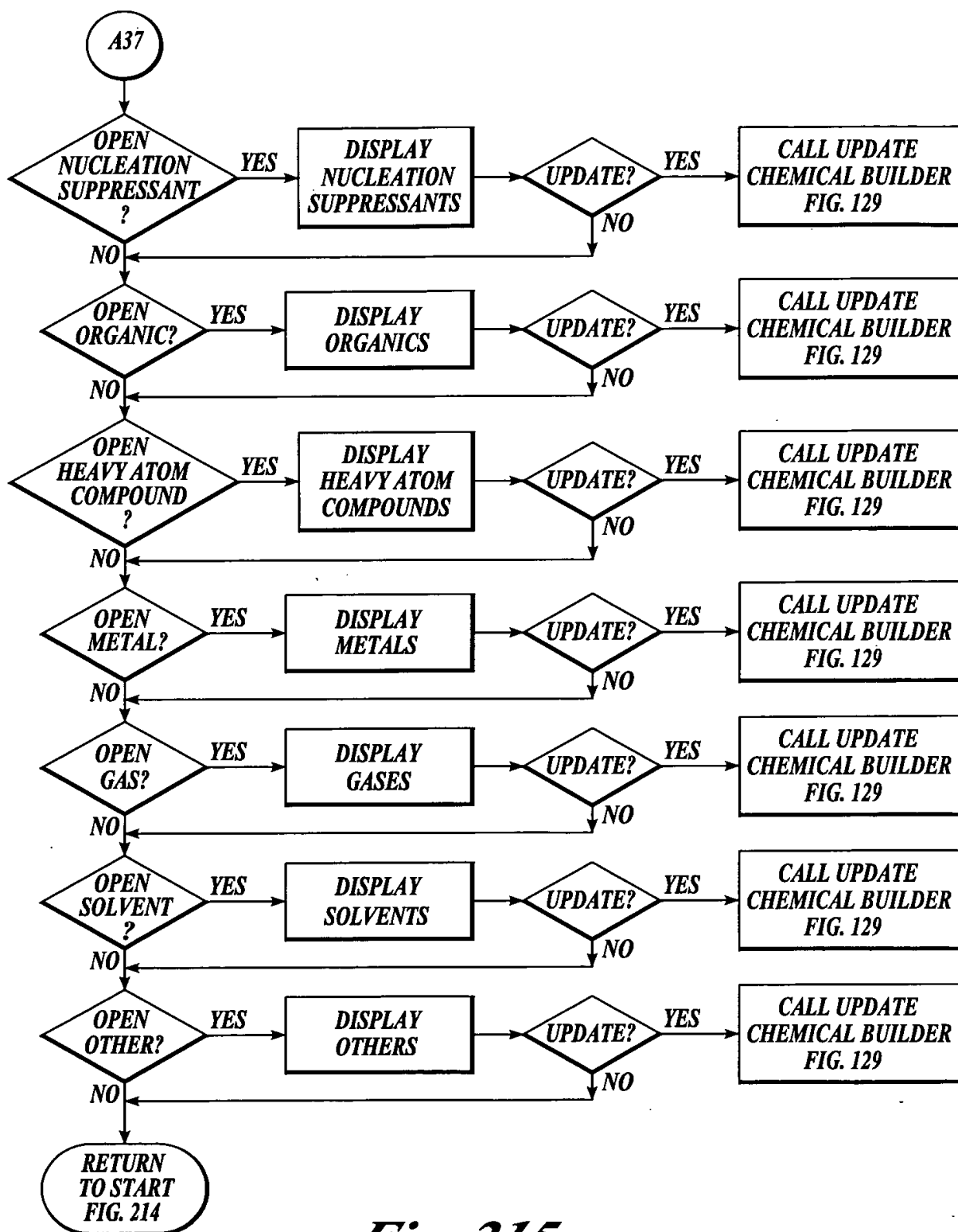
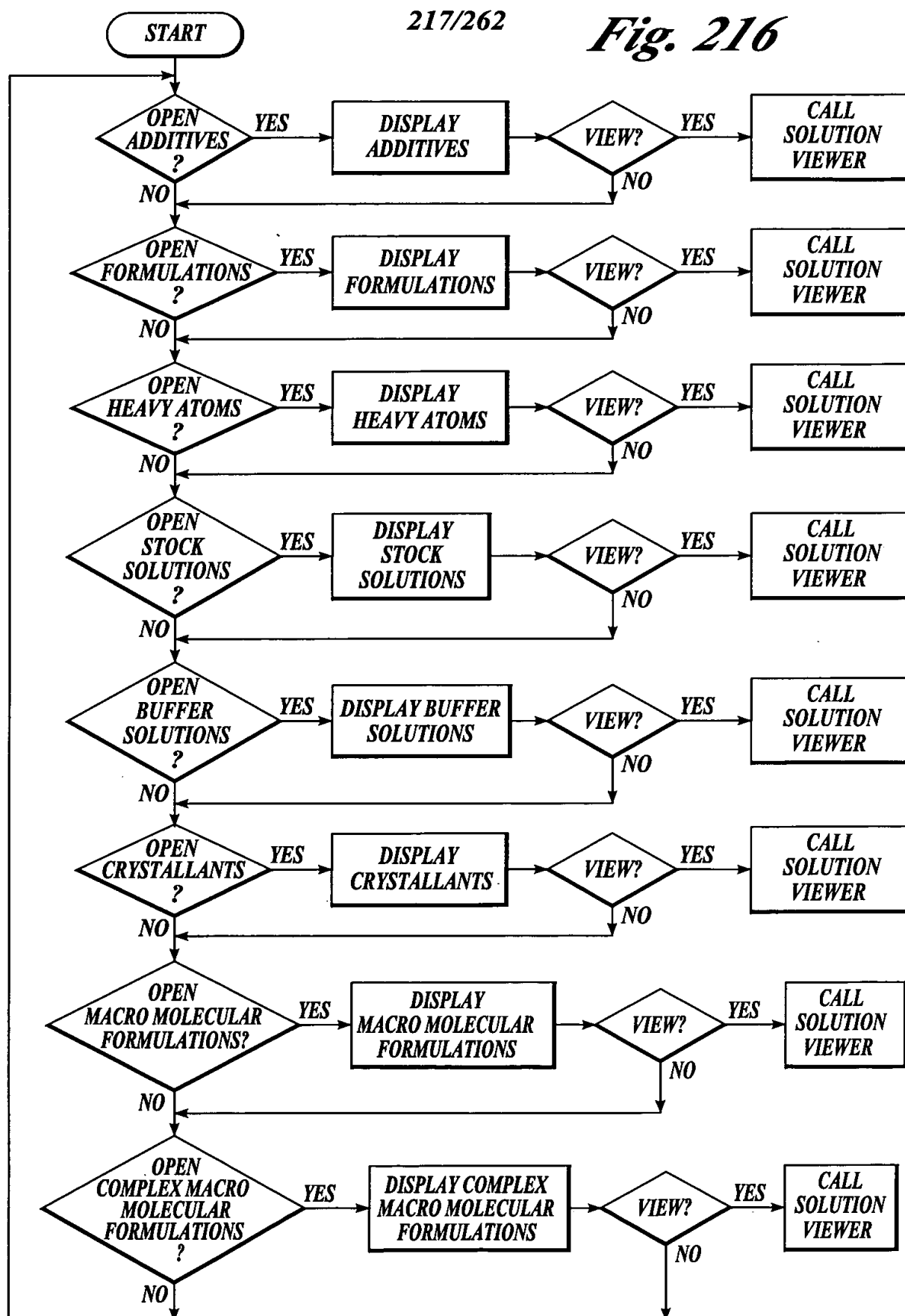


Fig. 212

*Fig. 213*

*Fig. 214*

*Fig. 215*



Database Object Manager

Crystal Monitor Objects:

- Base Objects
- Chemicals
 - Buffering Agent
 - pHConjugate
 - Precipitant
 - Salt
 - CSI
 - Chelator
 - Detergent
 - ReducingAgent
 - CryoCoolant
 - NucleationSuppressant
 - Organic
 - heavyAtomCompound
 - Metal
 - Gas
 - Solvent
 - Other
- Solutions

Attributes:

Catalog	CAS	ChemicalName	ShortName	F
20,781-0	151-50-8	potassium cyani...	KCN	K
78-1970	10025-99-7	potassium tetra...	K2PtCl4	K
F1502	103213-47-4	D-fructose 6-ph...	K2 D-fructose 6...	K
H7273	21799-87-1	hydroquinonesu...	K HQSA	C
HR2-539	6381-59-5	potassium/sodiu...	K/Na tartrate	K
HR2-553	7778-77-0	potassium dihyd...	K H2 phosphate	K
HR2-635	7758-11-4	di-potassium hy...	K2 H phosphate	K
P0165	6381-59-5	potassium sodiu...	K/Na tartrate	C
P0662	7778-77-0	potassium phos...	K H2 phosphate	K
P2569	7789-23-3	potassium fluoride	KF	K
P2713	333-20-0	potassium thioc...	KSCN	K
P3786	7758-11-4	potassium phos...	K2 H phosphate	K
P5708	127-08-2	potassium acetate	KAc	K
P9333	7447-40-7	potassium chlori...	KCl	K
P9458	7779-80-5	potassium sulfate	K2 sulfate	K
T6897	921-53-9	potassium tartrate	K2 tartrate	K

select * from chemicals where chemicalName like '%potass%';

Execute SQL Query

16 rows. Query time: 361 ms

Help...

Fig. 217

21700

Database Object Manager

Crystal Monitor Objects:

- Base Objects
- Chemicals
 - Buffering Agent
 - pHConjugate
 - Precipitant
 - Salt
 - CSI
 - Chelator
 - Detergent
 - ReducingAgent
 - CryoCoolant
 - NucleationSuppressant
 - Organic
 - heavyAtomCompound
 - Metal
 - Gas
 - Solvent
 - Other
- Solutions

Attributes:

Catalog	CAS	ChemicalName	ShortName
A7330	631-61-8	ammonium acet...	NH4 aC
HR2-565	631-61-8	ammonium acet...	NH4 aC
A6141	1066-33-7	ammonium bicar...	NH4 bicarbonate
A5666	12125-02-9	ammonium chlori...	NH4 chloride
HR2-555	7722-76-1	ammonium dihyd...	NH4 H2 phosph...
F2004	540-69-2	ammonium form...	NH3 formate
A7455	6484-52-2	ammonium nitrate	NH4 nitrate
A1167	7783-28-0	ammonium phos...	(NH4)2 H phosph...
A2939	7783-20-2	ammonium sulfate	(NH4)2 sulfate
A938-500	7783-20-2	ammonium sulfate	(NH4)2 sulfate
HR2-541	7783-20-2	ammonium sulfate	(NH4)2 sulfate
JT0792-5	7783-20-2	ammonium sulfate	(NH4)2 sulfate
HR2-567	10035-04-8	calcium chloride...	CaCl2
C4705	62-54-4	calcium acetate	CaAc2
HR2-567	62-54-4	calcium acetate	CaAc2
C5080	10035-04-8	calcium chloride...	CaCl2

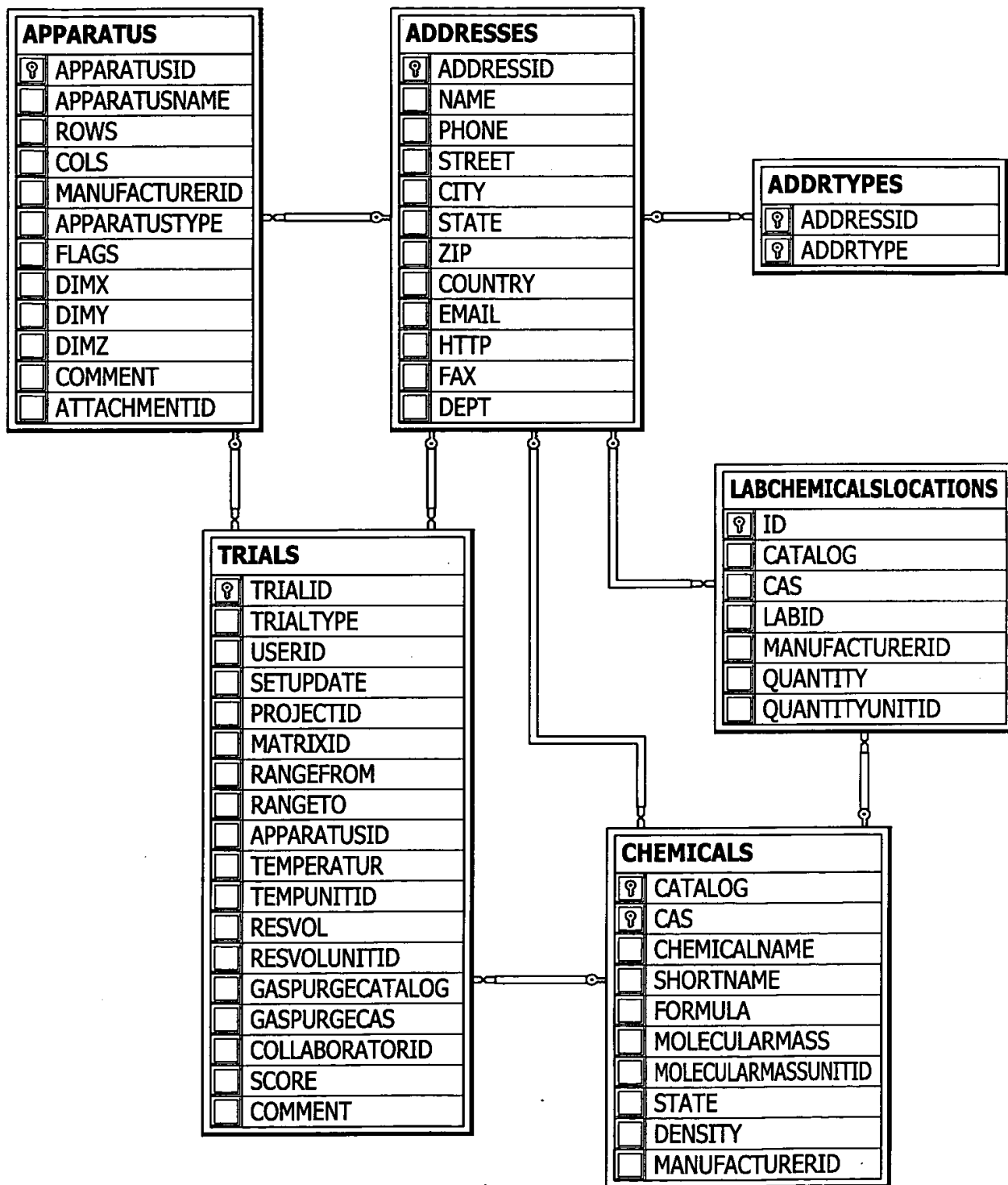
Execute SQL Query

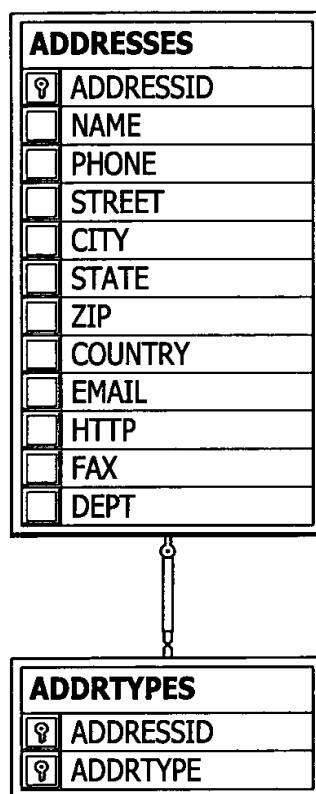
77 rows. Query time: 81 ms

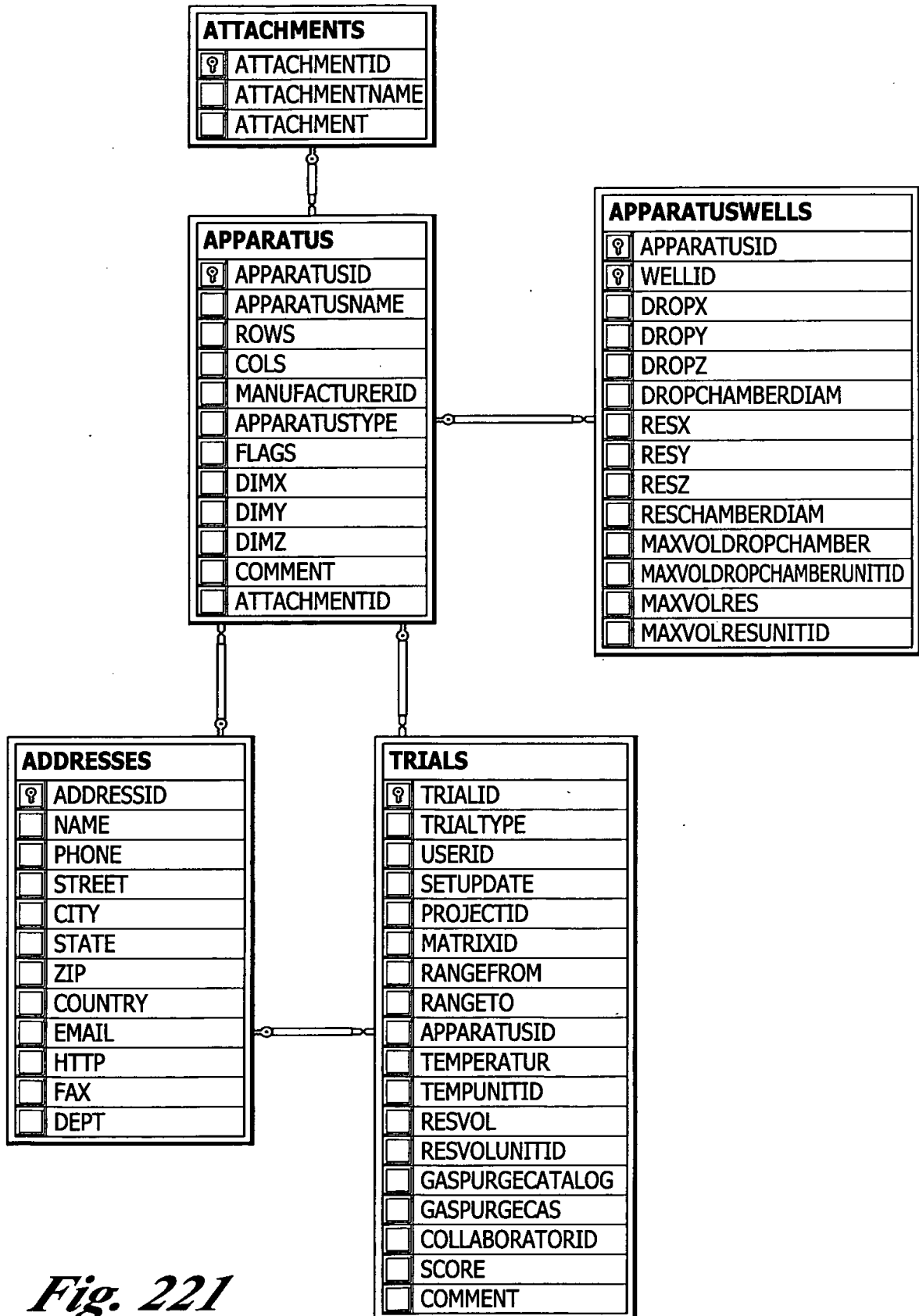
Help...

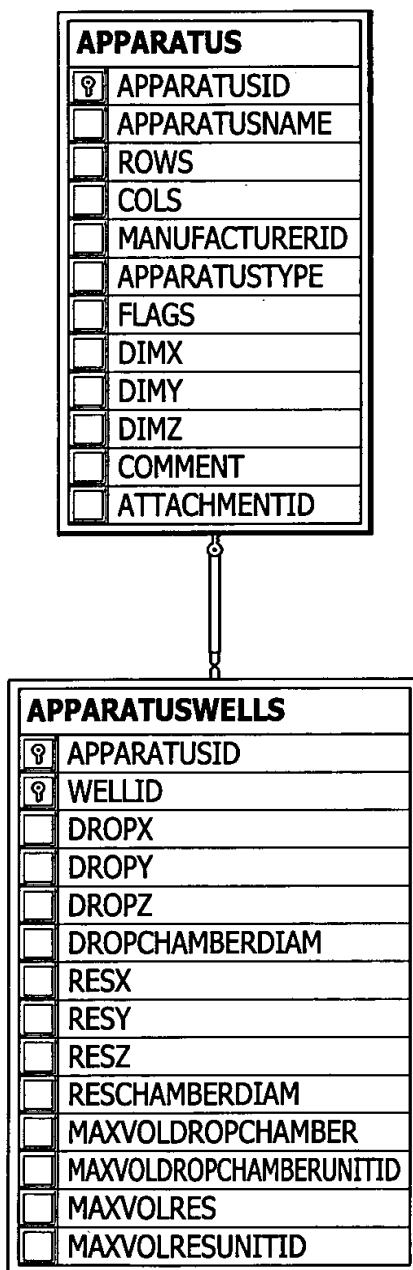
21800

Fig. 218

*Fig. 219*

*Fig. 220*

*Fig. 221*

*Fig. 222*

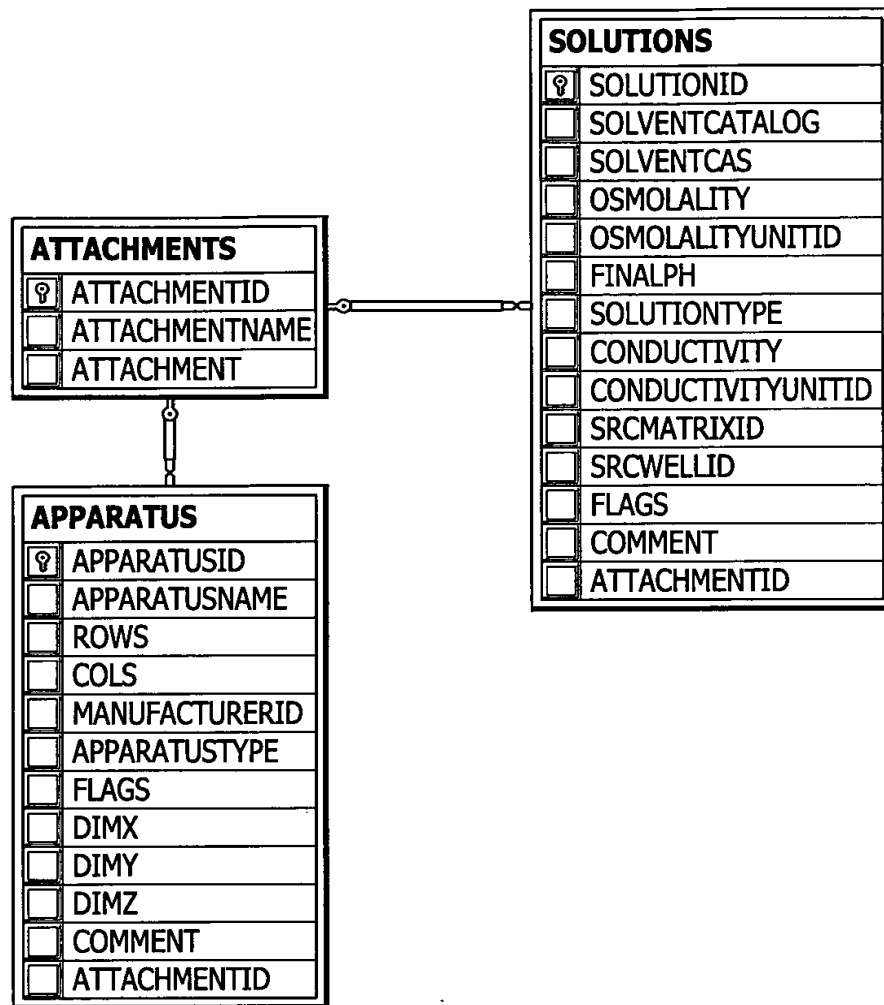
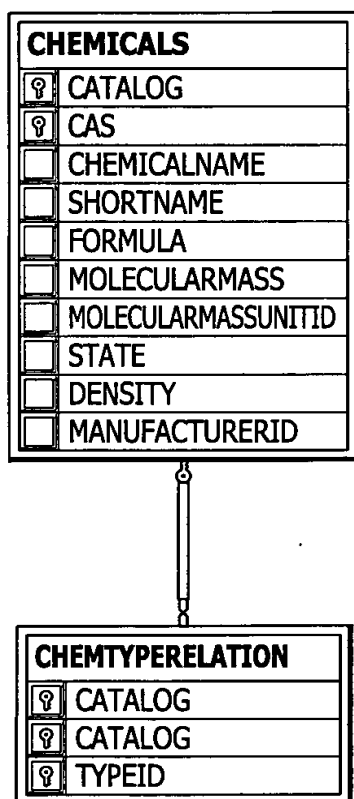
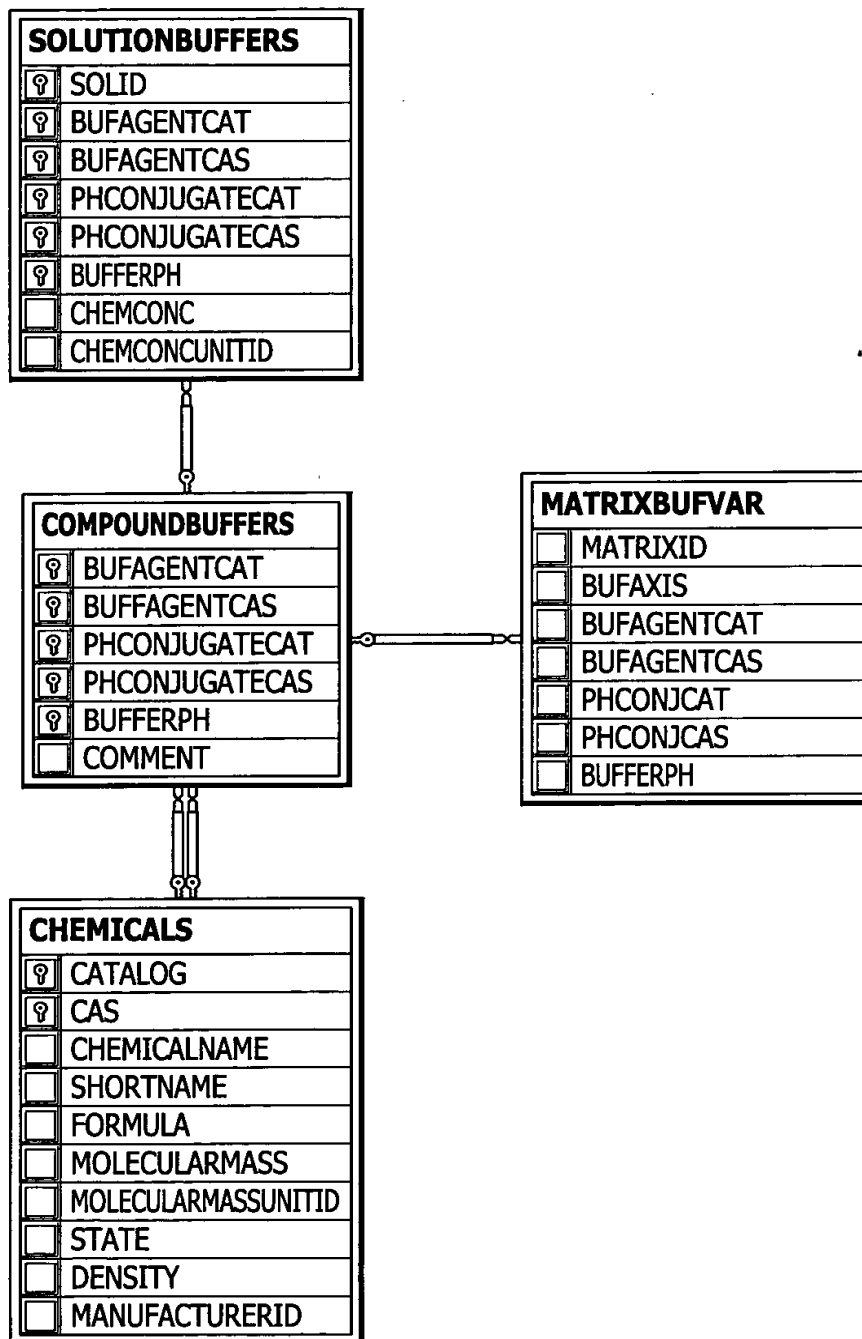
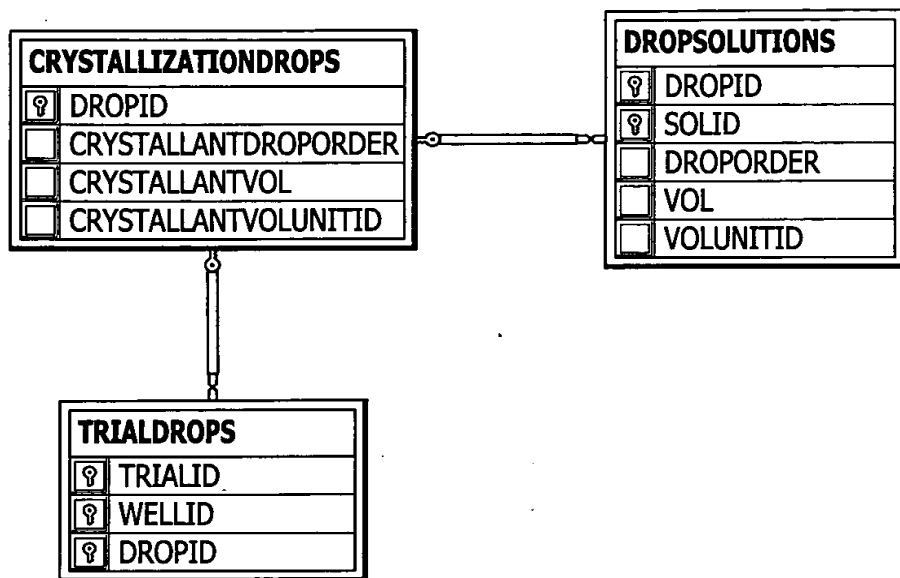
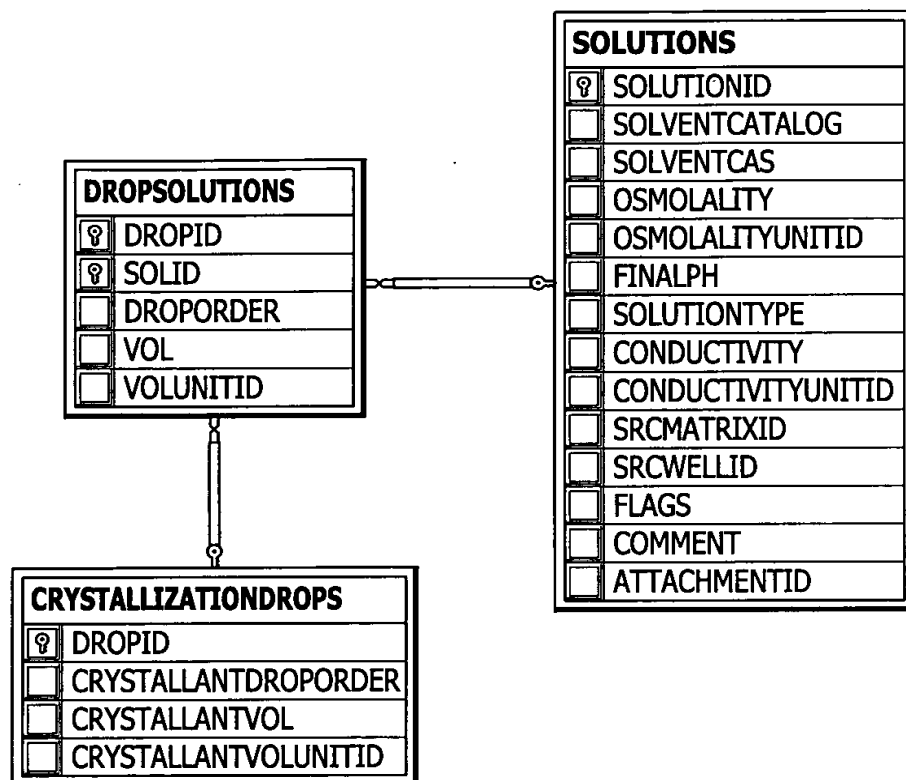
*Fig. 223*

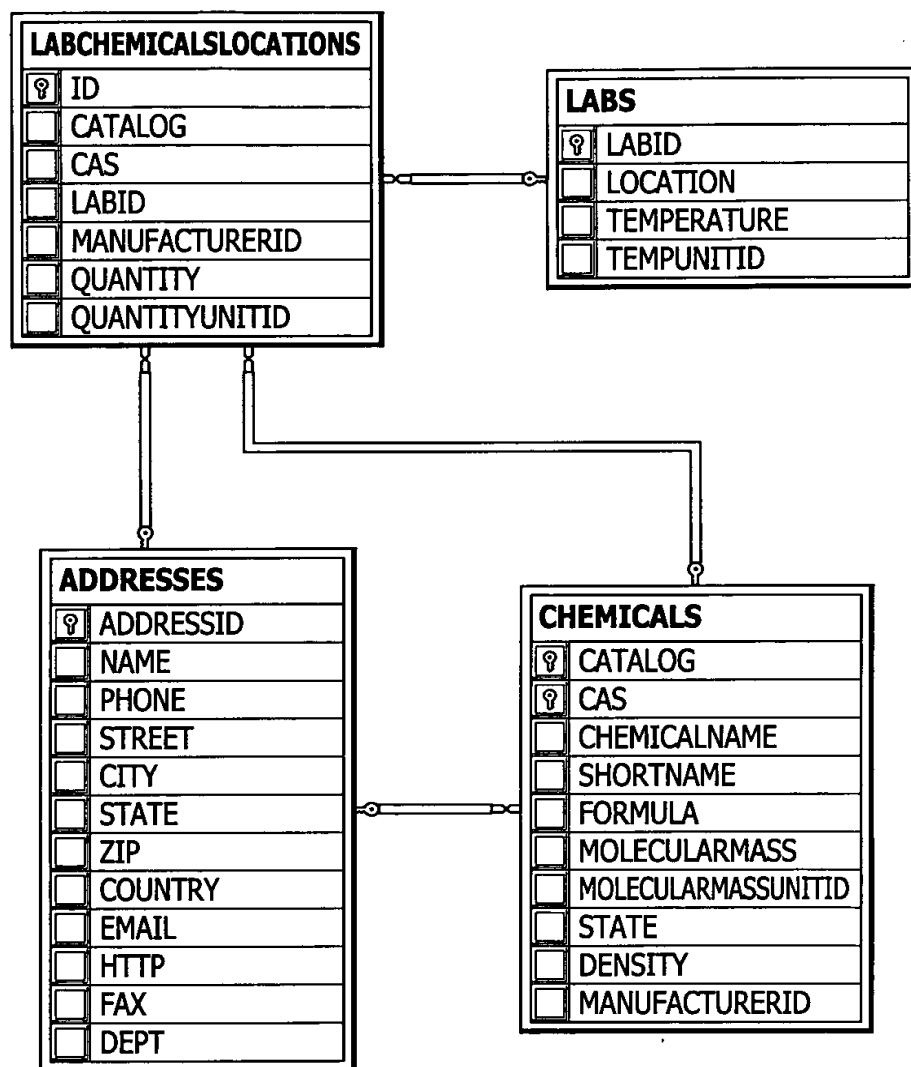
Fig. 224

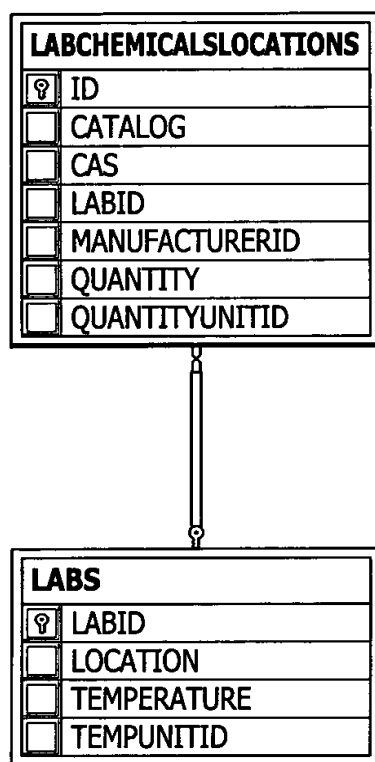
*Fig. 225*

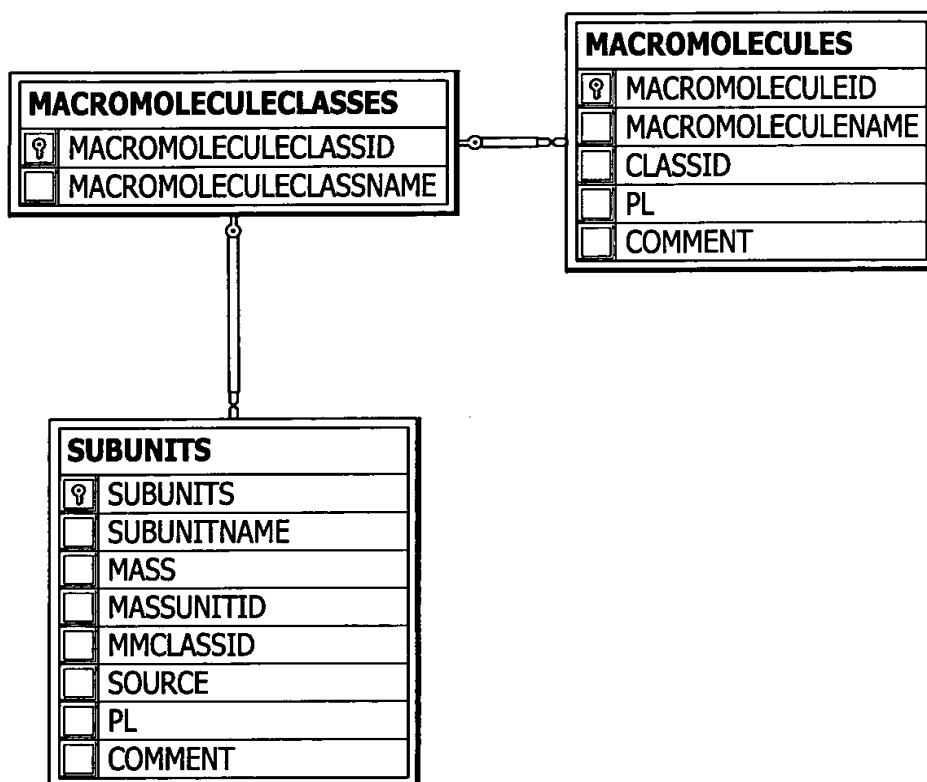
*Fig. 226*

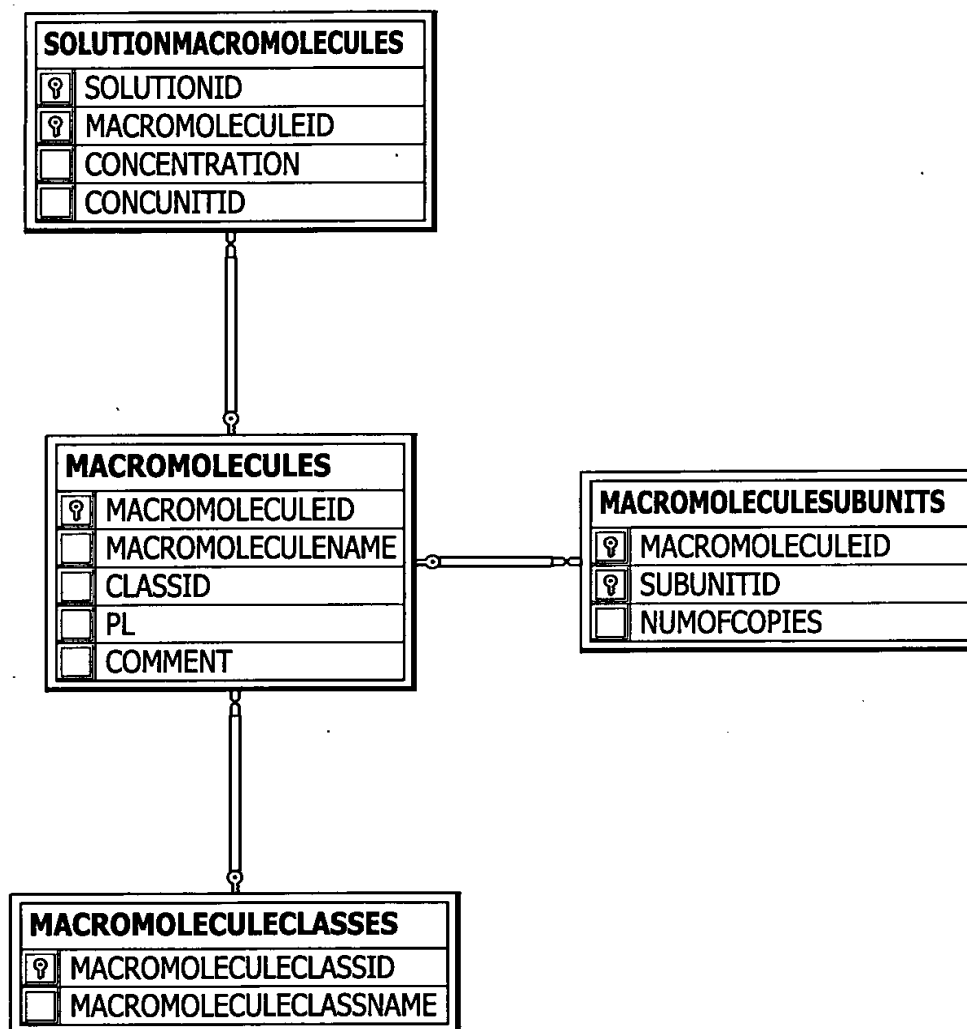
*Fig. 227*

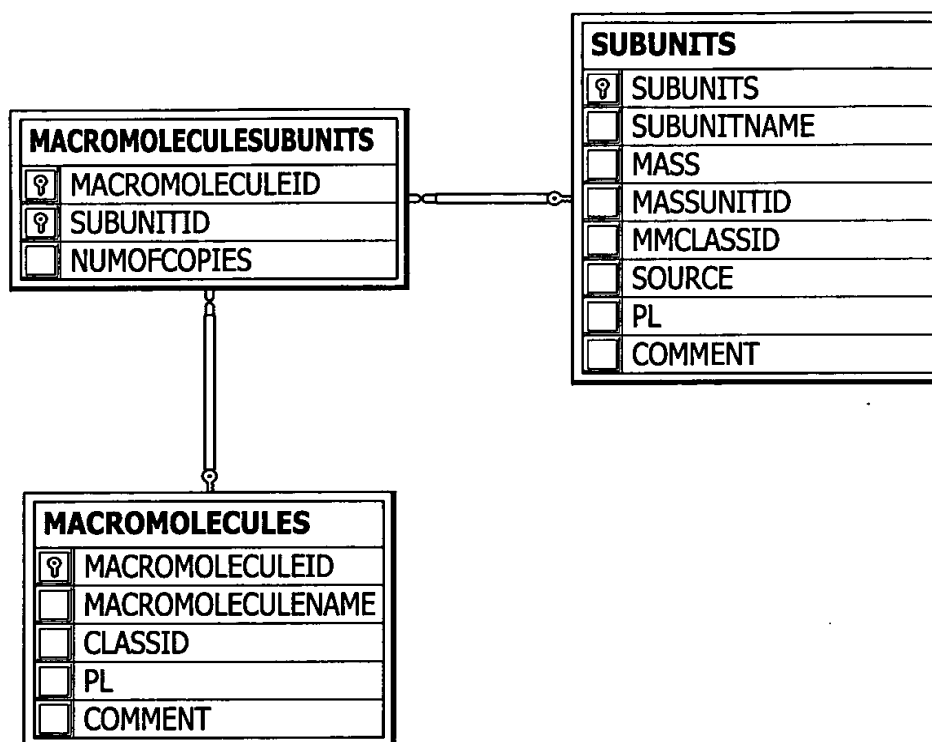
*Fig. 228*

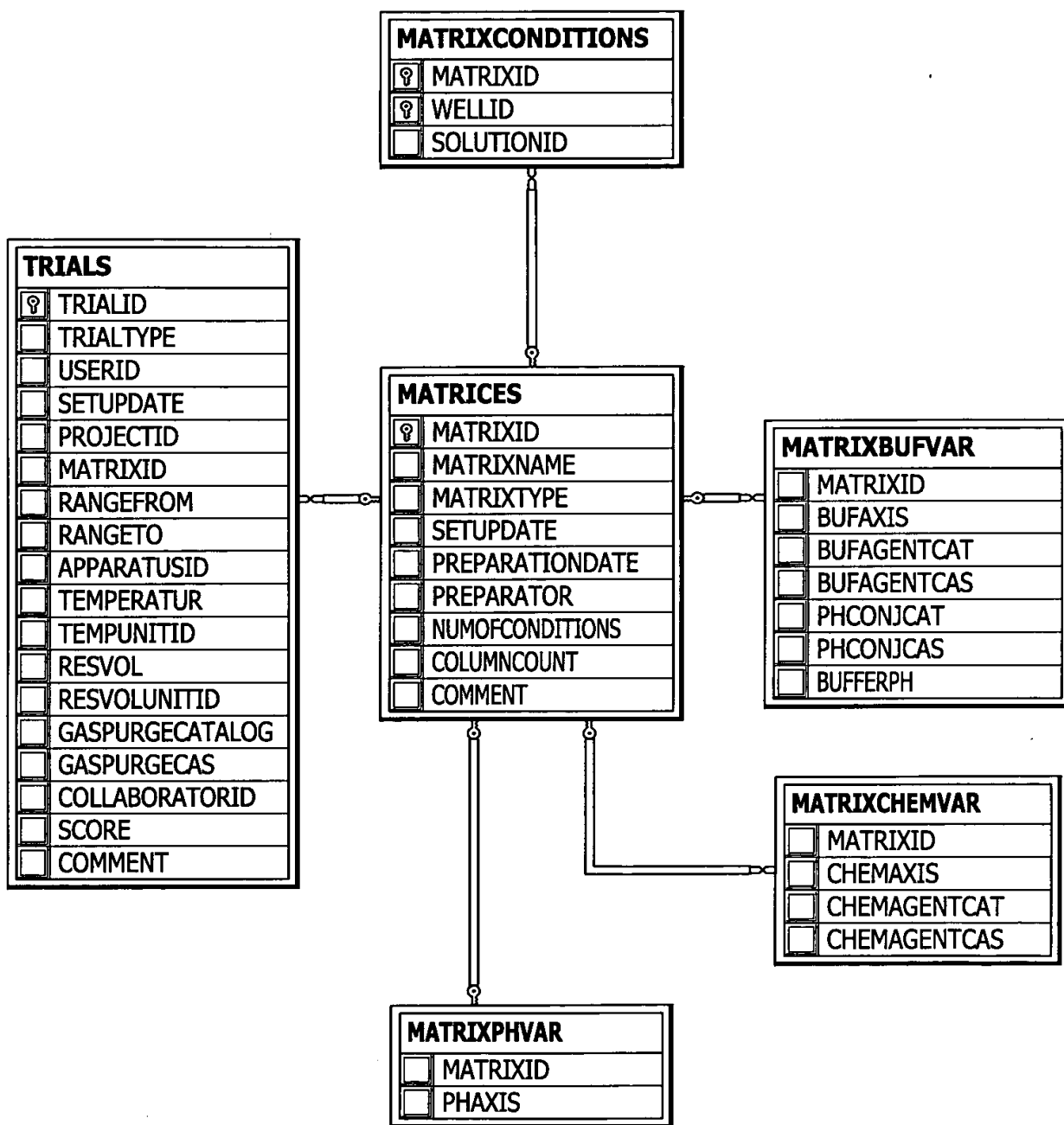
*Fig. 229*

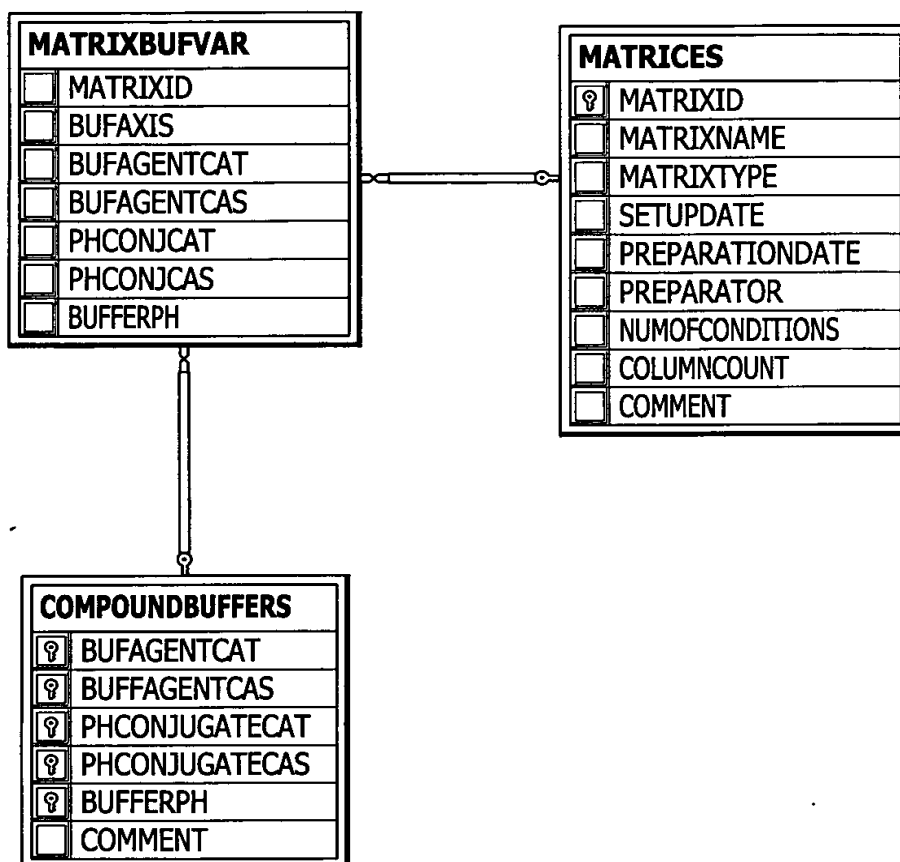
*Fig. 230*

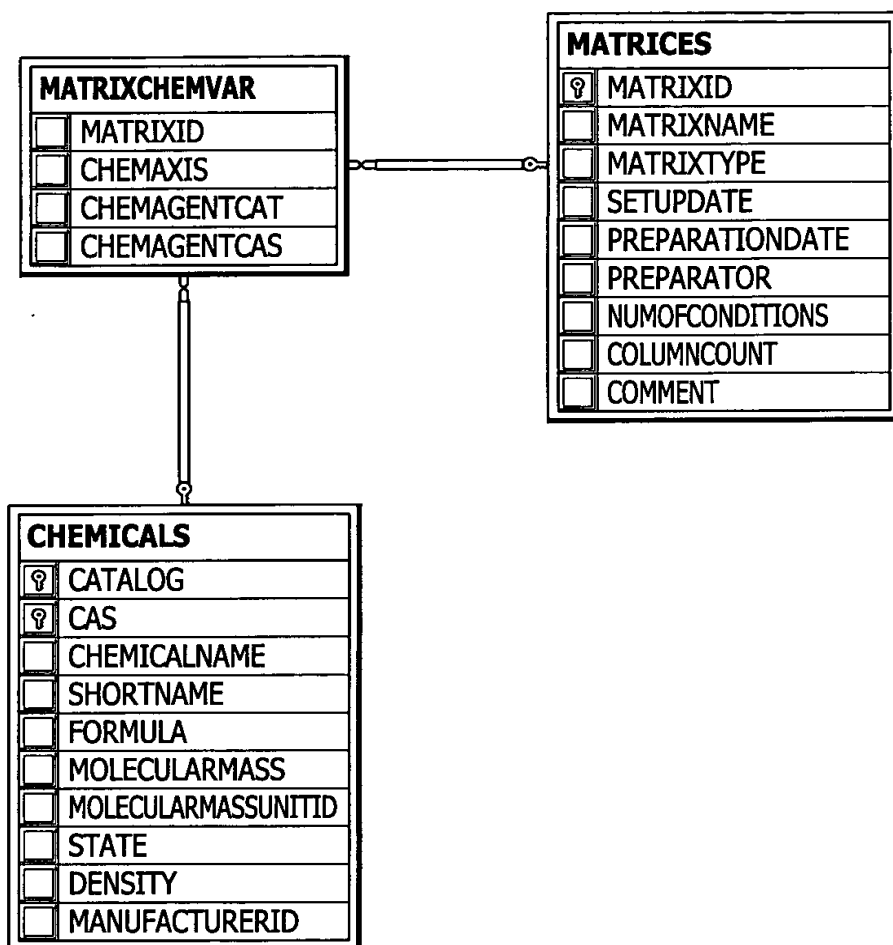
*Fig. 231*

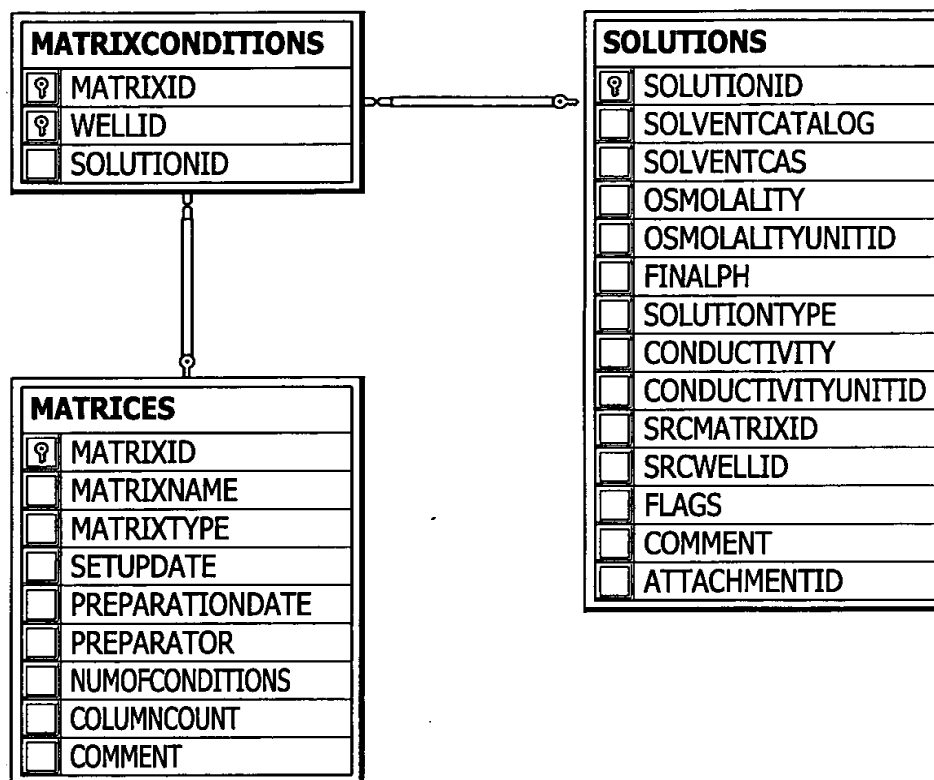
*Fig. 232*

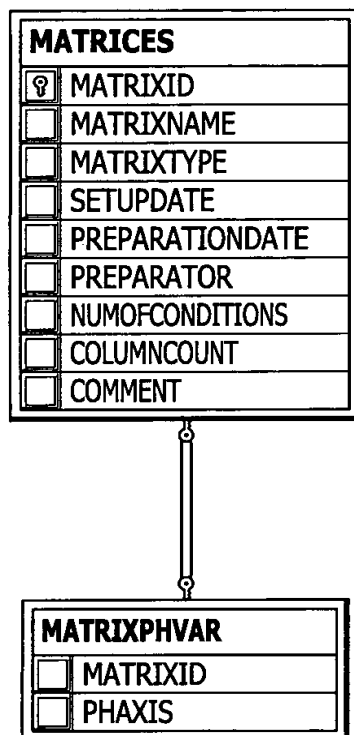
*Fig. 233*

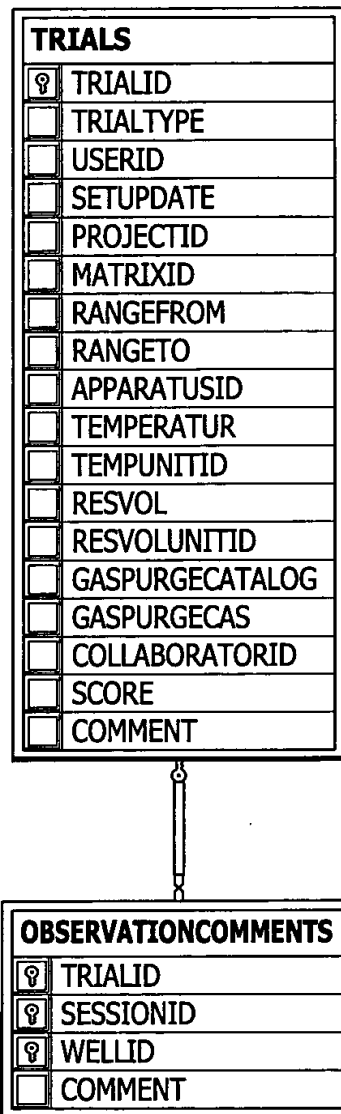
*Fig. 234*

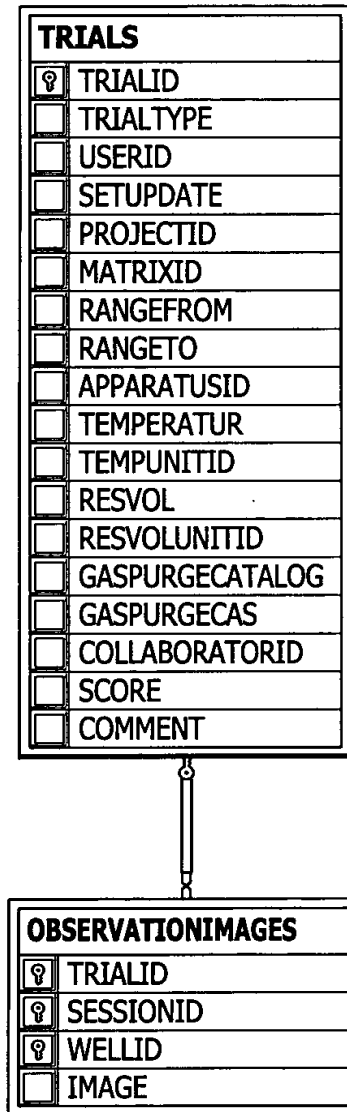
*Fig. 235*

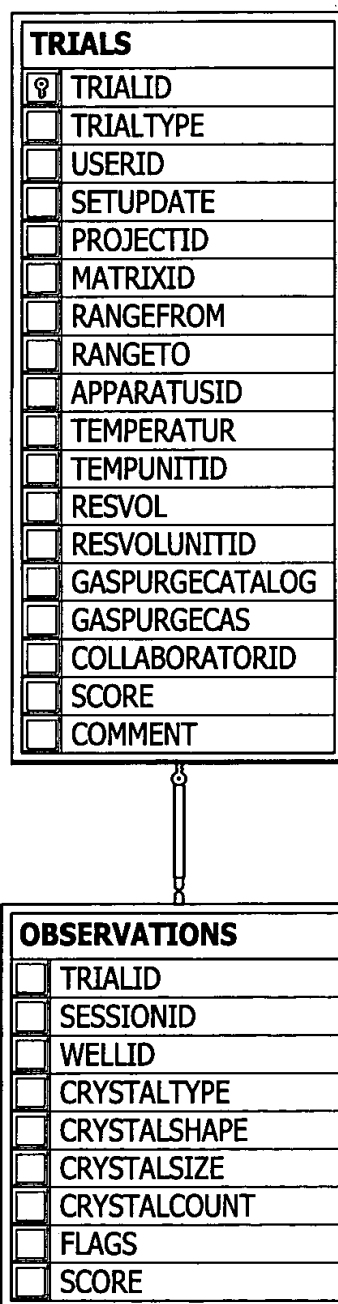
*Fig. 236*

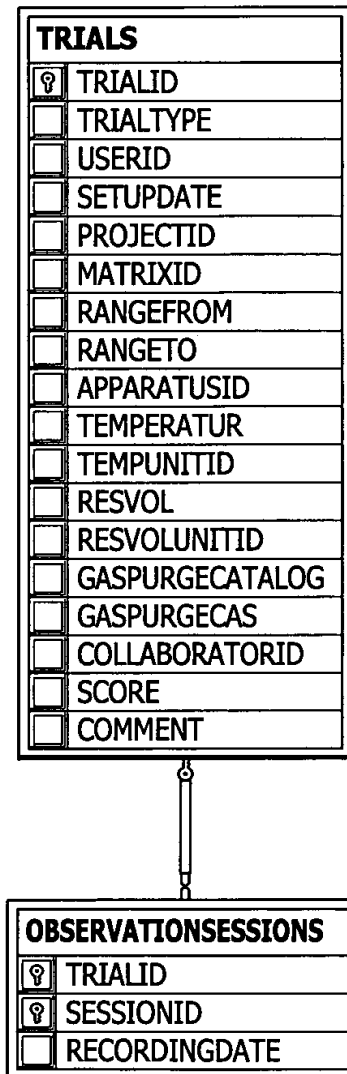
*Fig. 237*

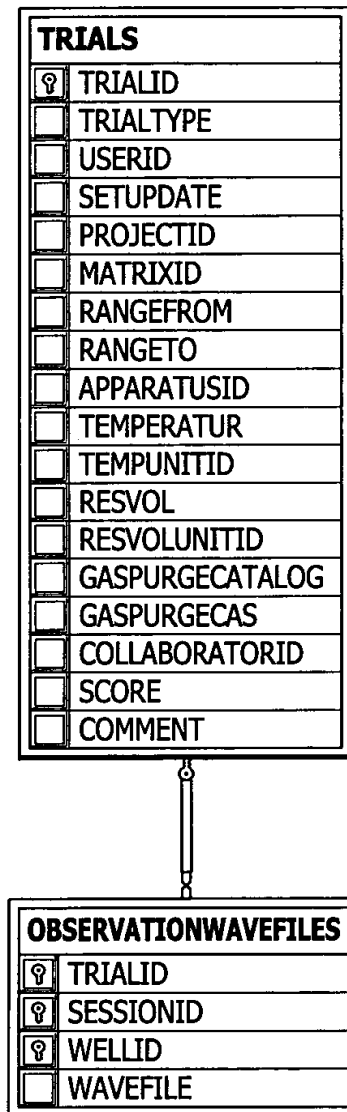
*Fig. 238*

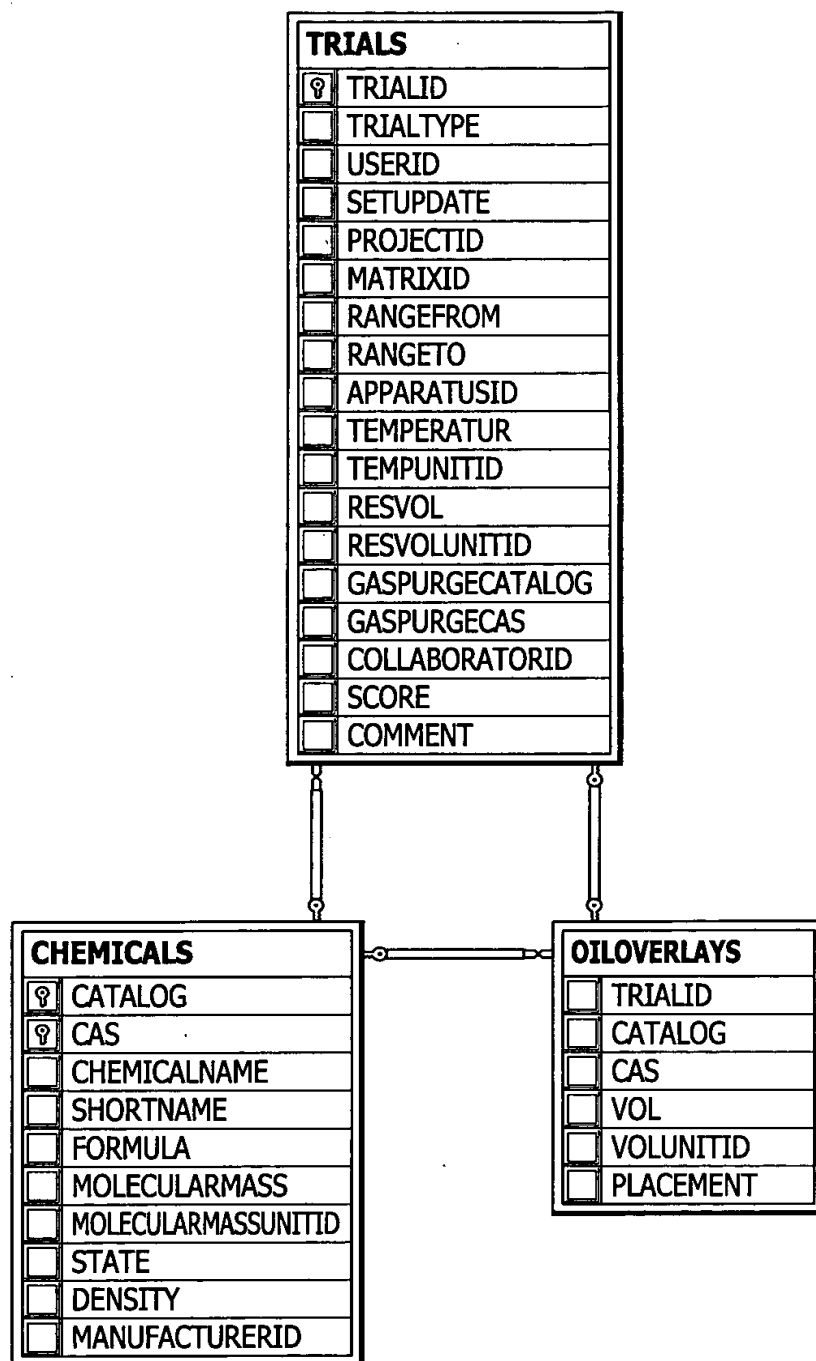
*Fig. 239*

*Fig. 240*

*Fig. 241*

*Fig. 242*

*Fig. 243*

*Fig. 244*

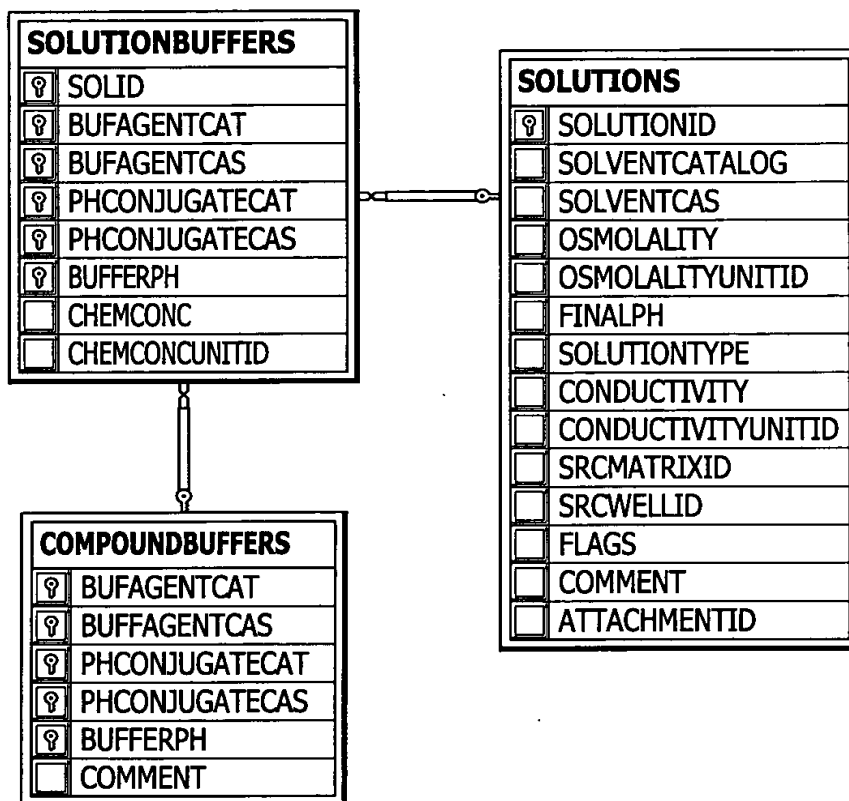
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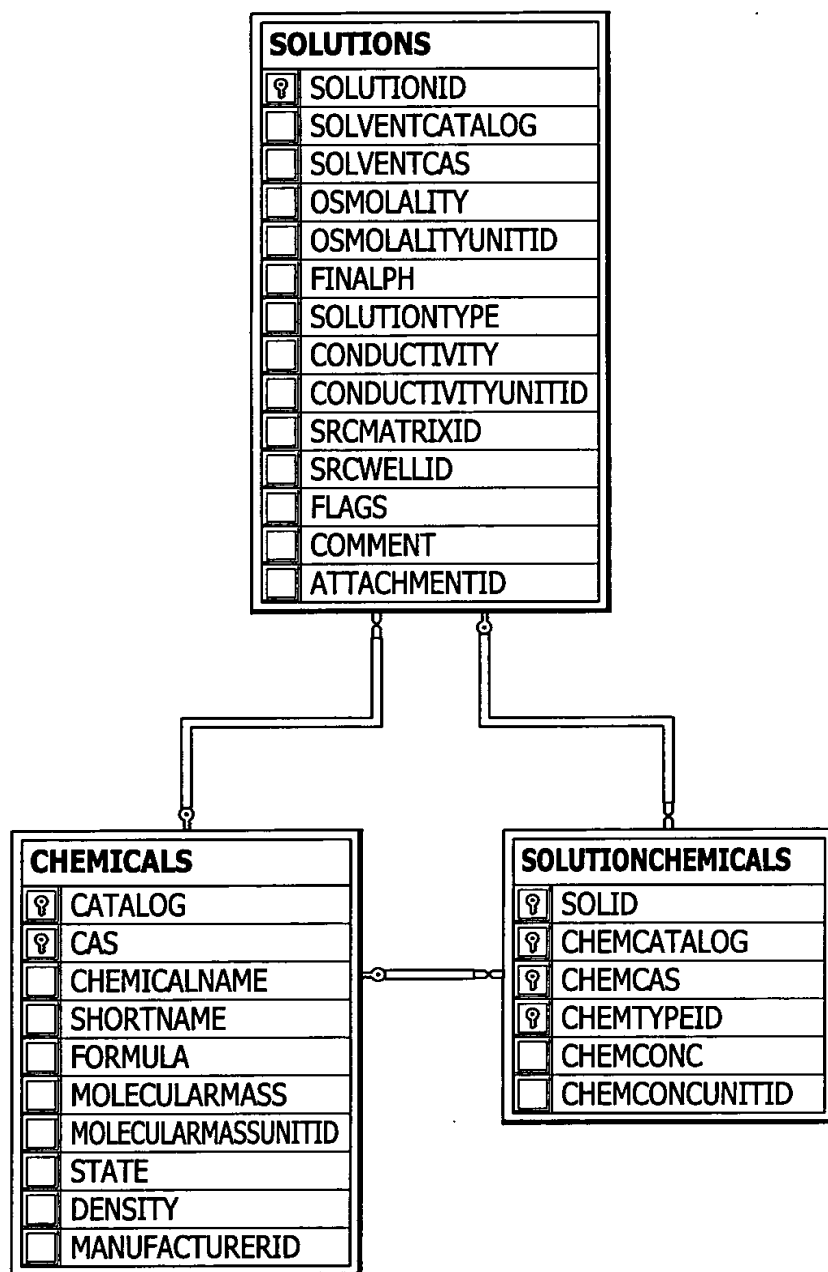
Fig. 245

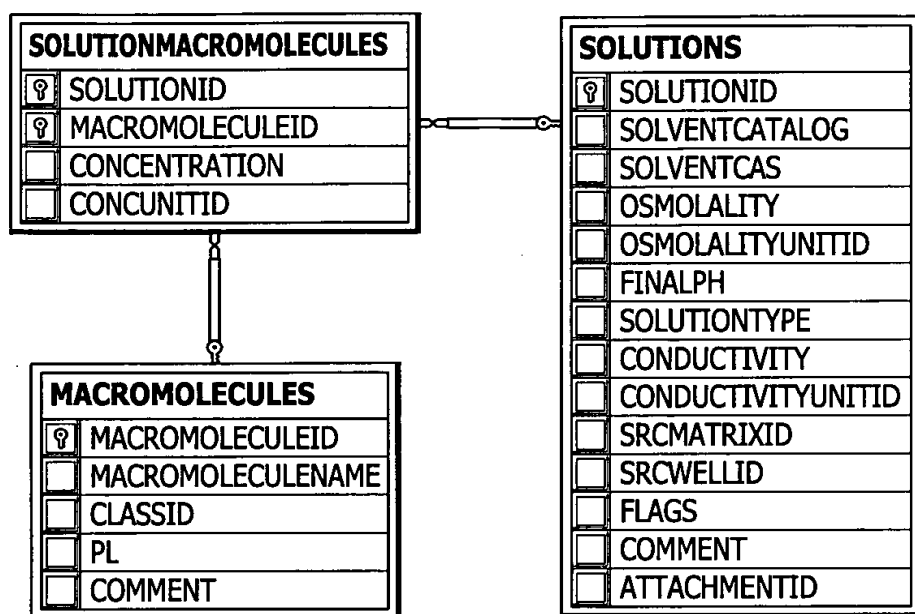
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<input type="checkbox"/>	RANGETO
<input type="checkbox"/>	APPARATUSID
<input type="checkbox"/>	TEMPERATUR
<input type="checkbox"/>	TEMPUNITID
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<input type="checkbox"/>	RESVOLUNITID
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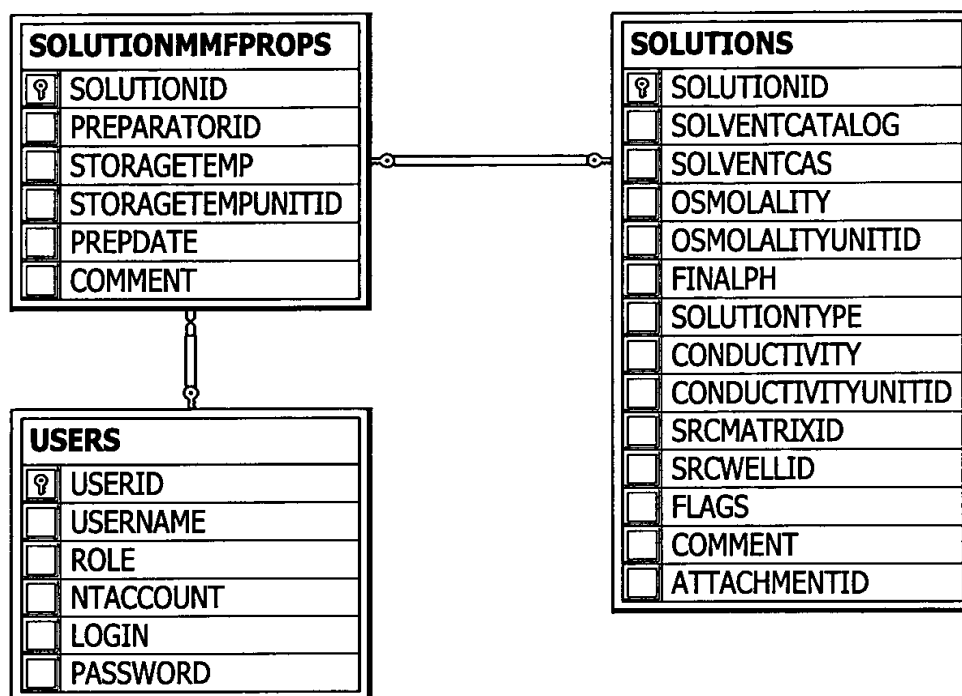
Fig. 246

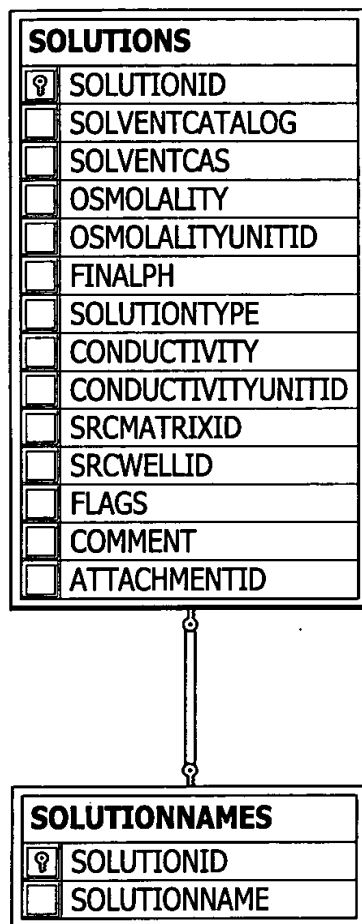
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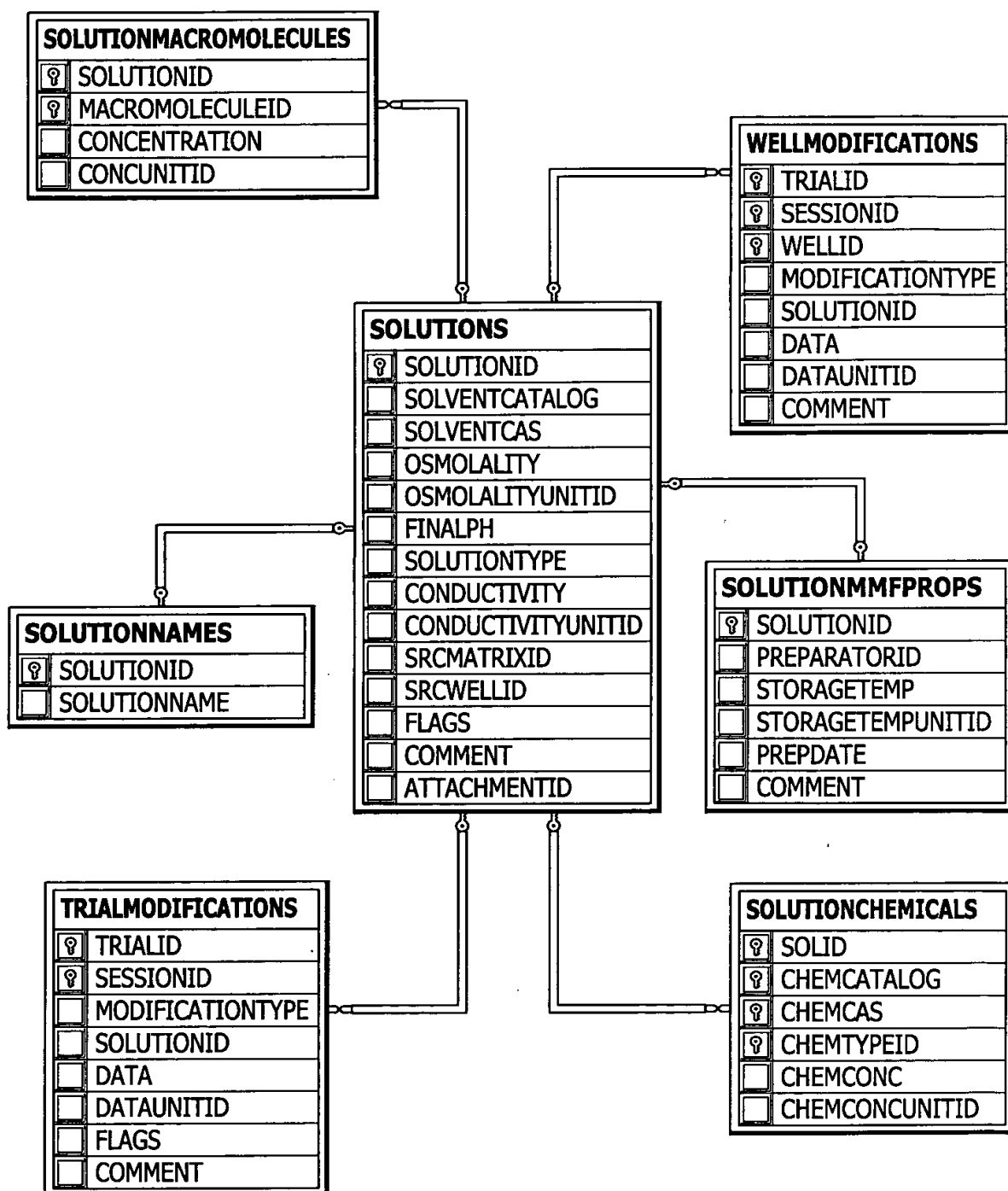
*Fig. 247*

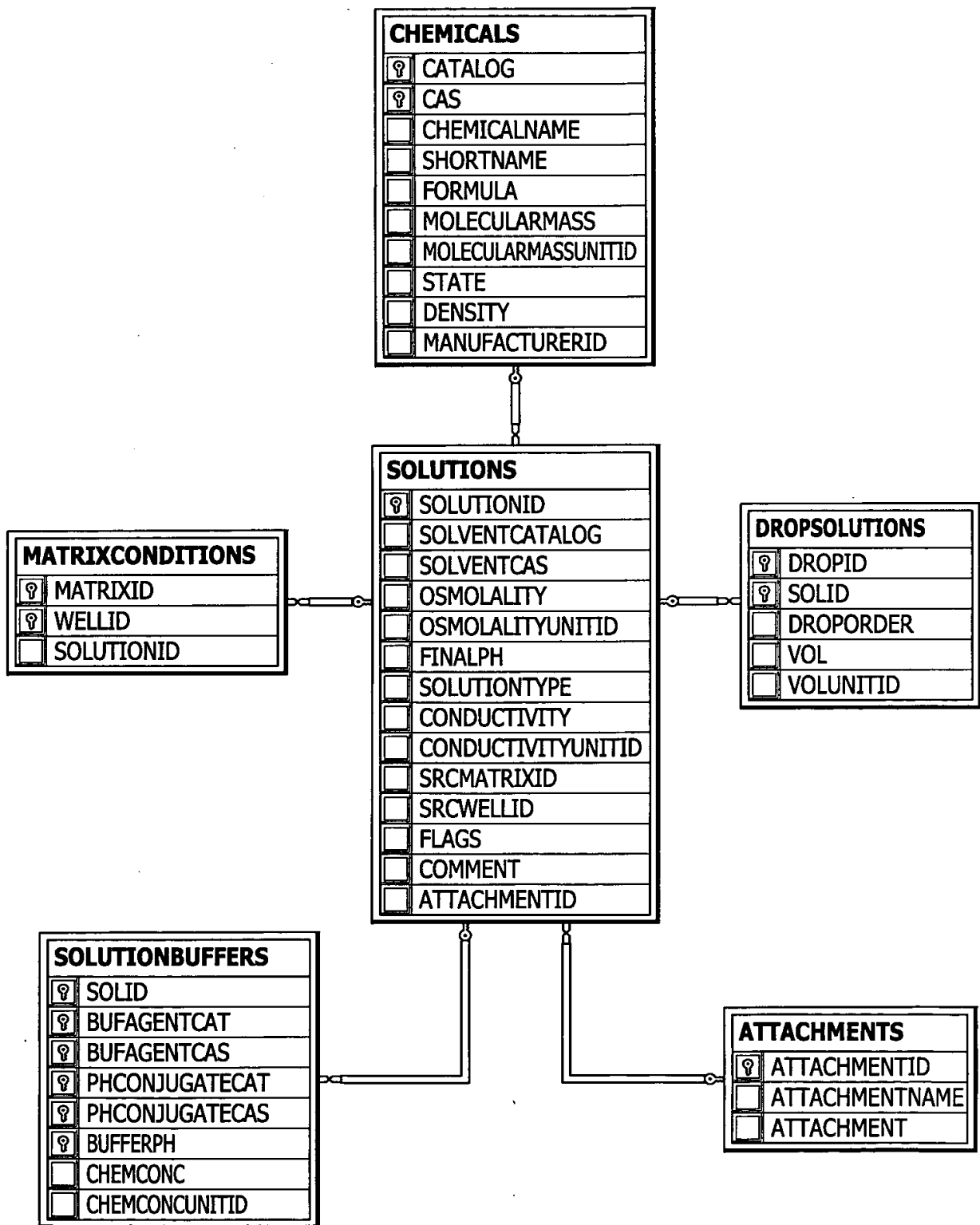
*Fig. 248*

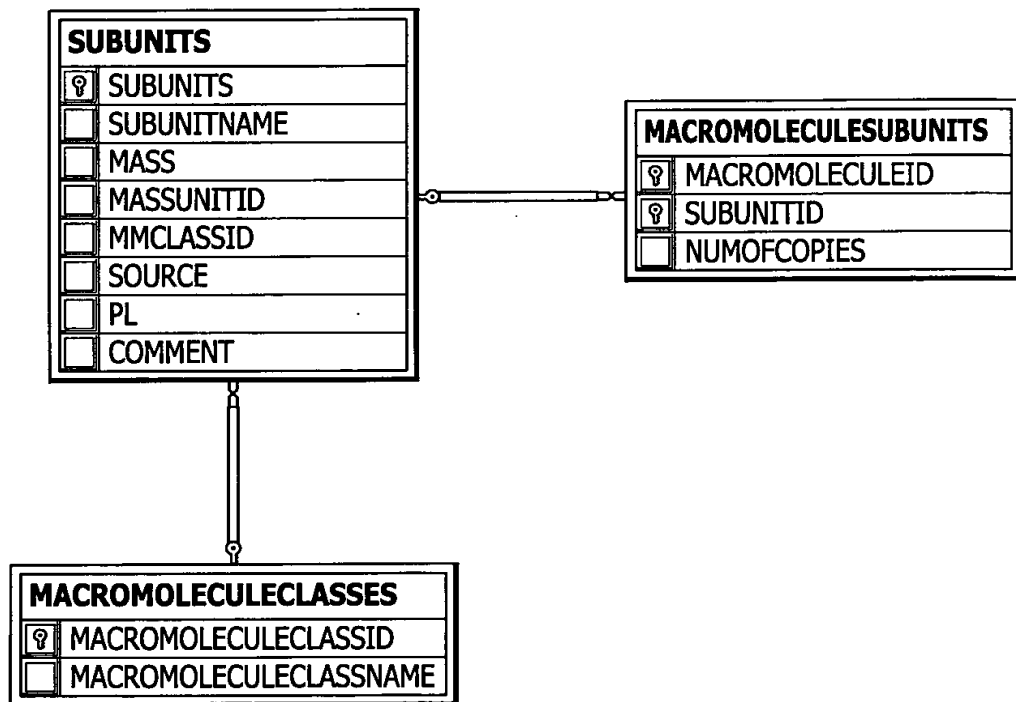
*Fig. 249*

*Fig. 250*

*Fig. 251*

*Fig. 252*

*Fig. 253*

*Fig. 254*

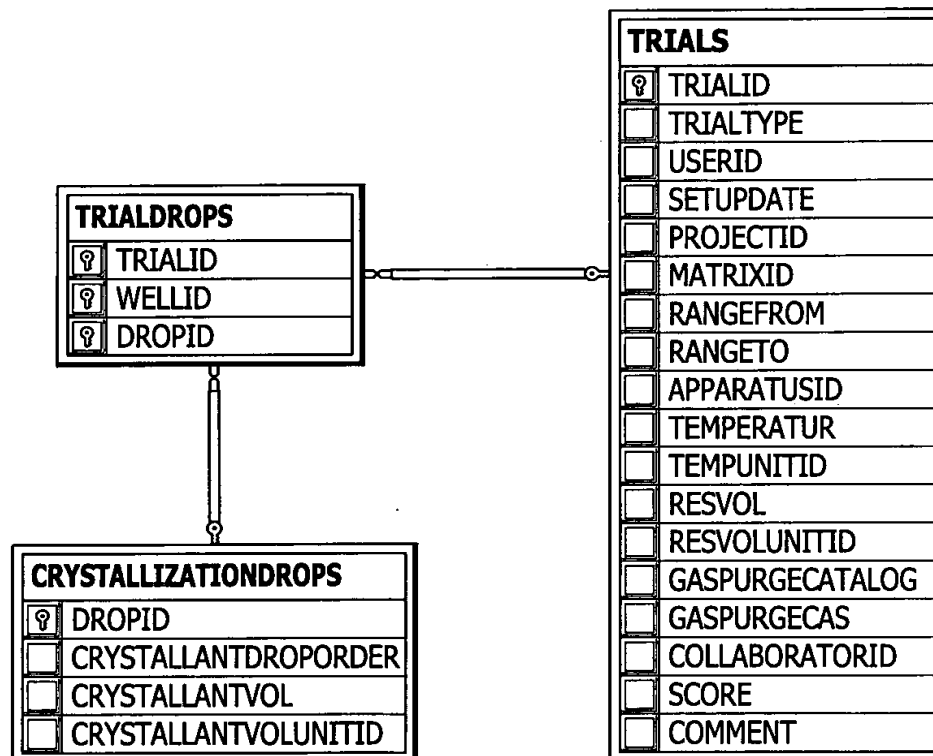
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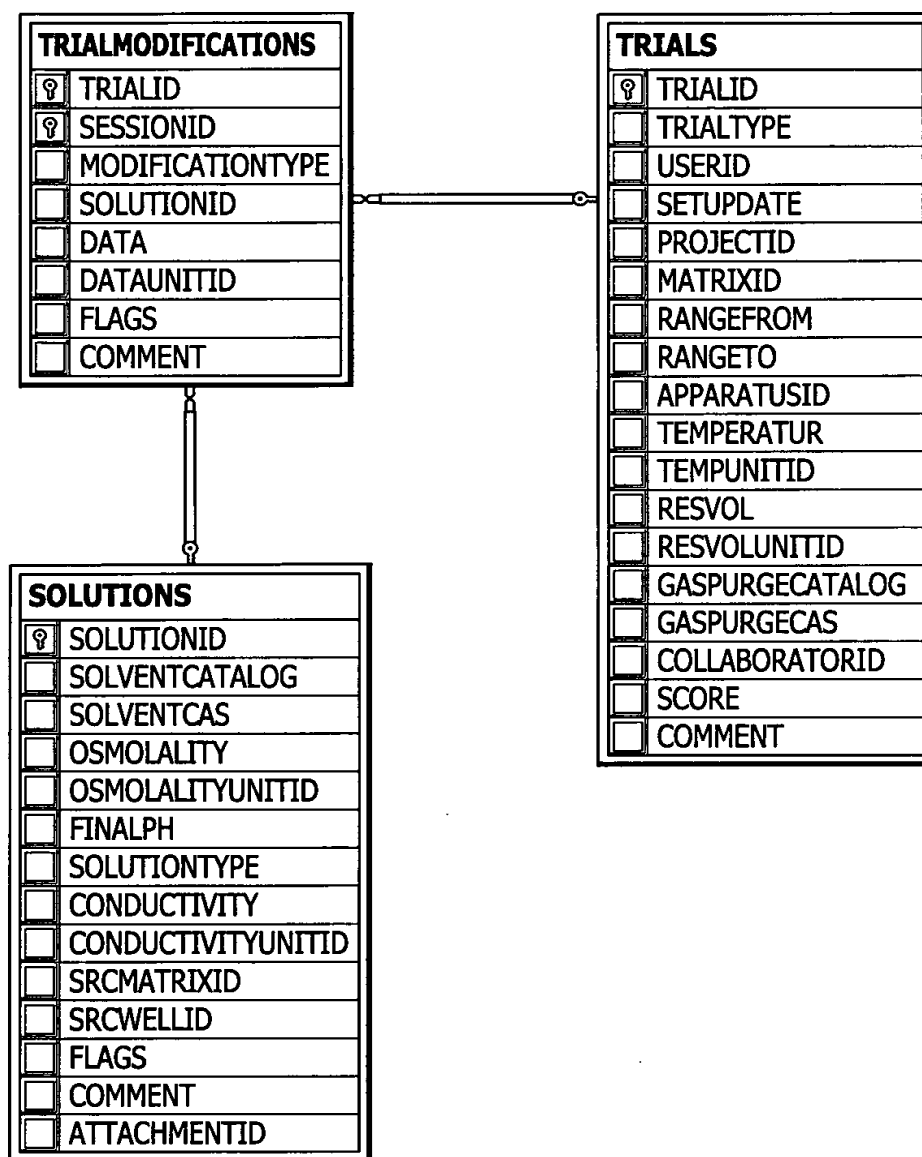
Fig. 255

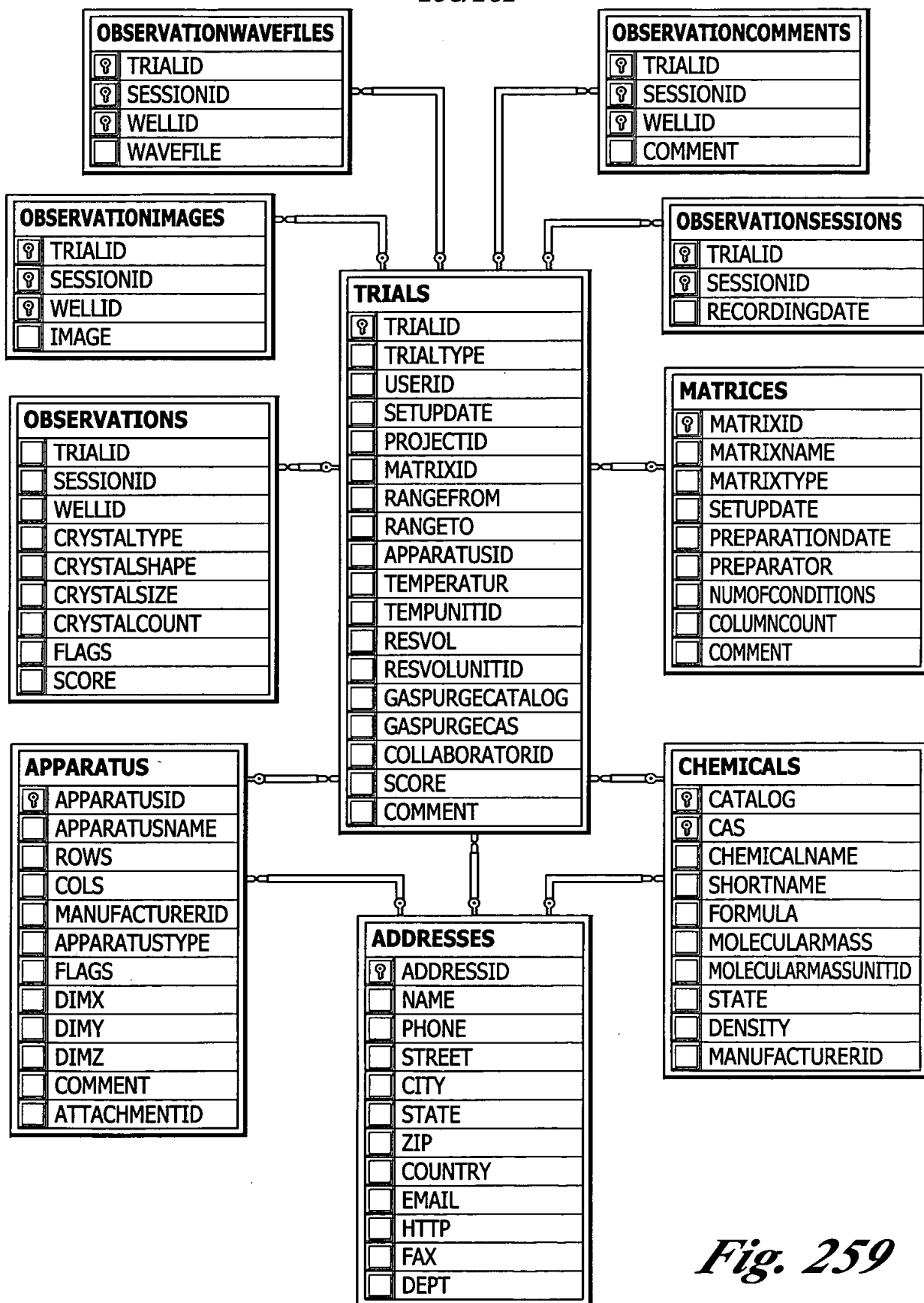
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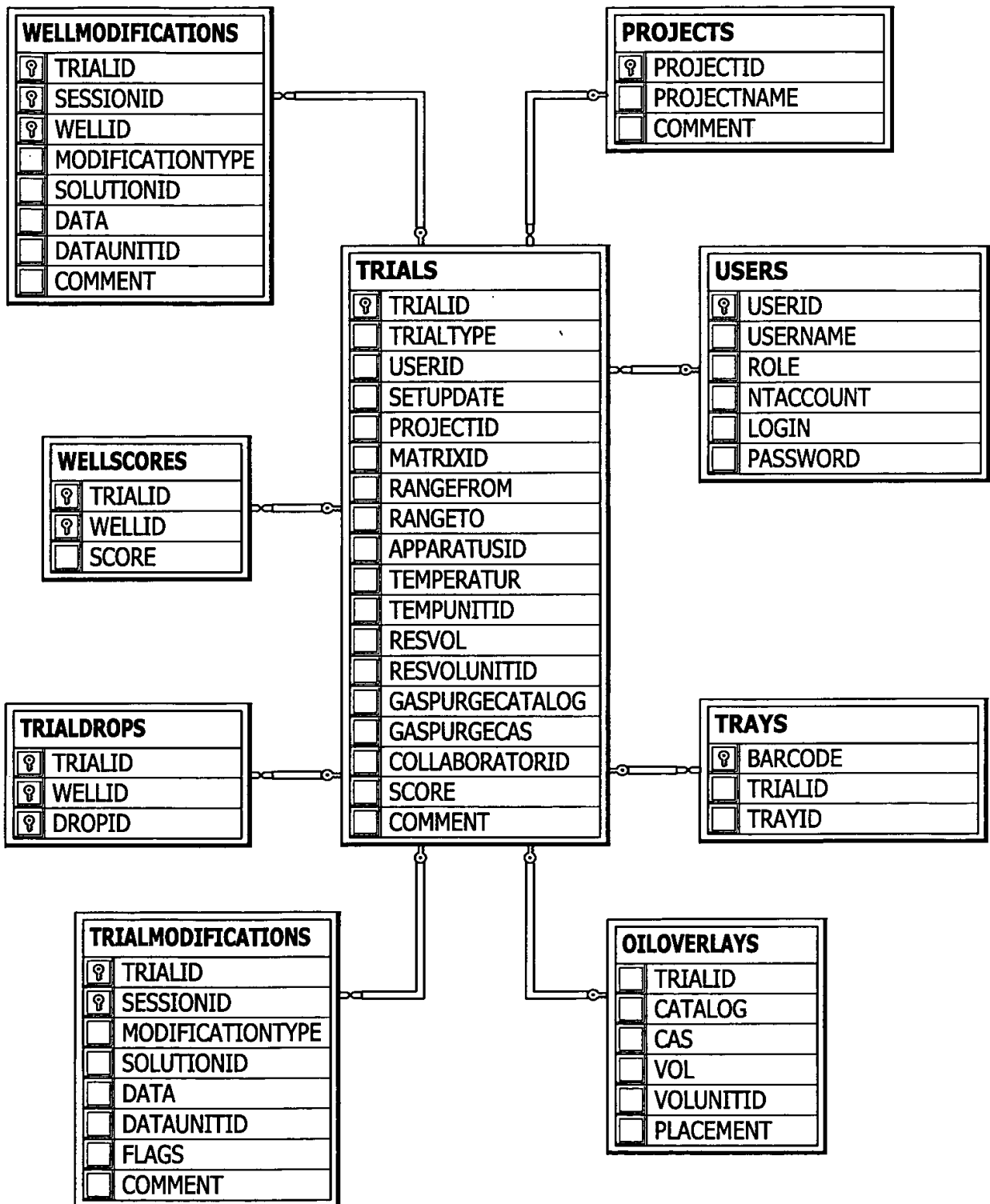
Fig. 256

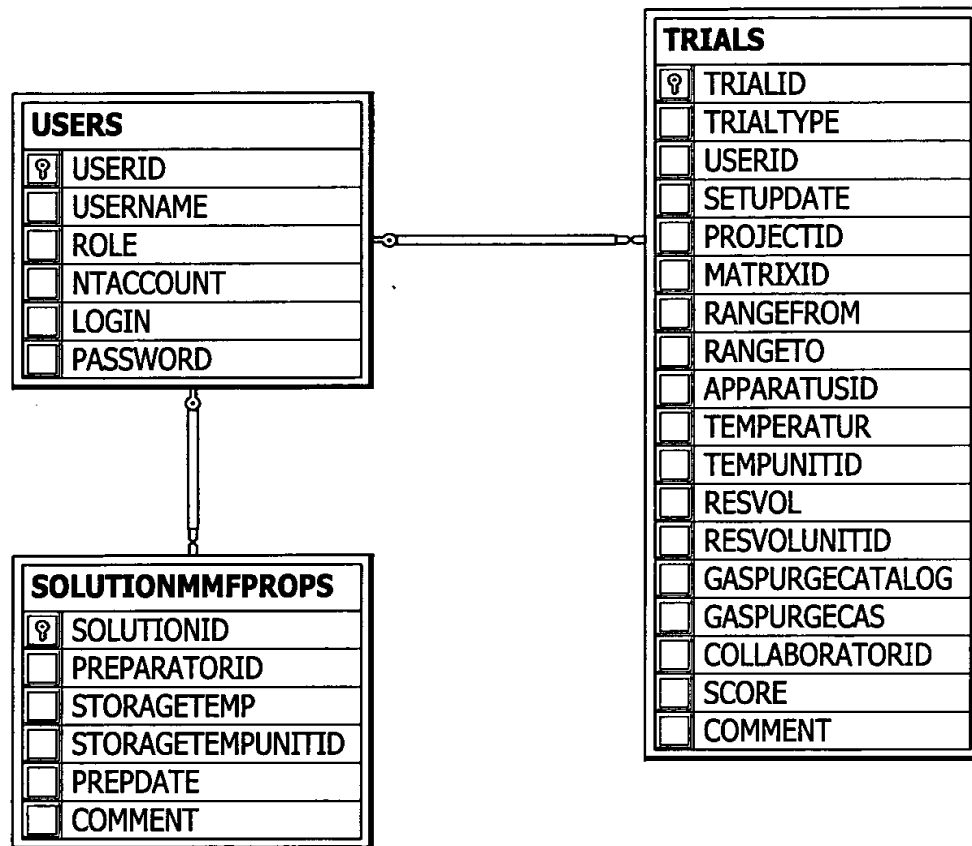
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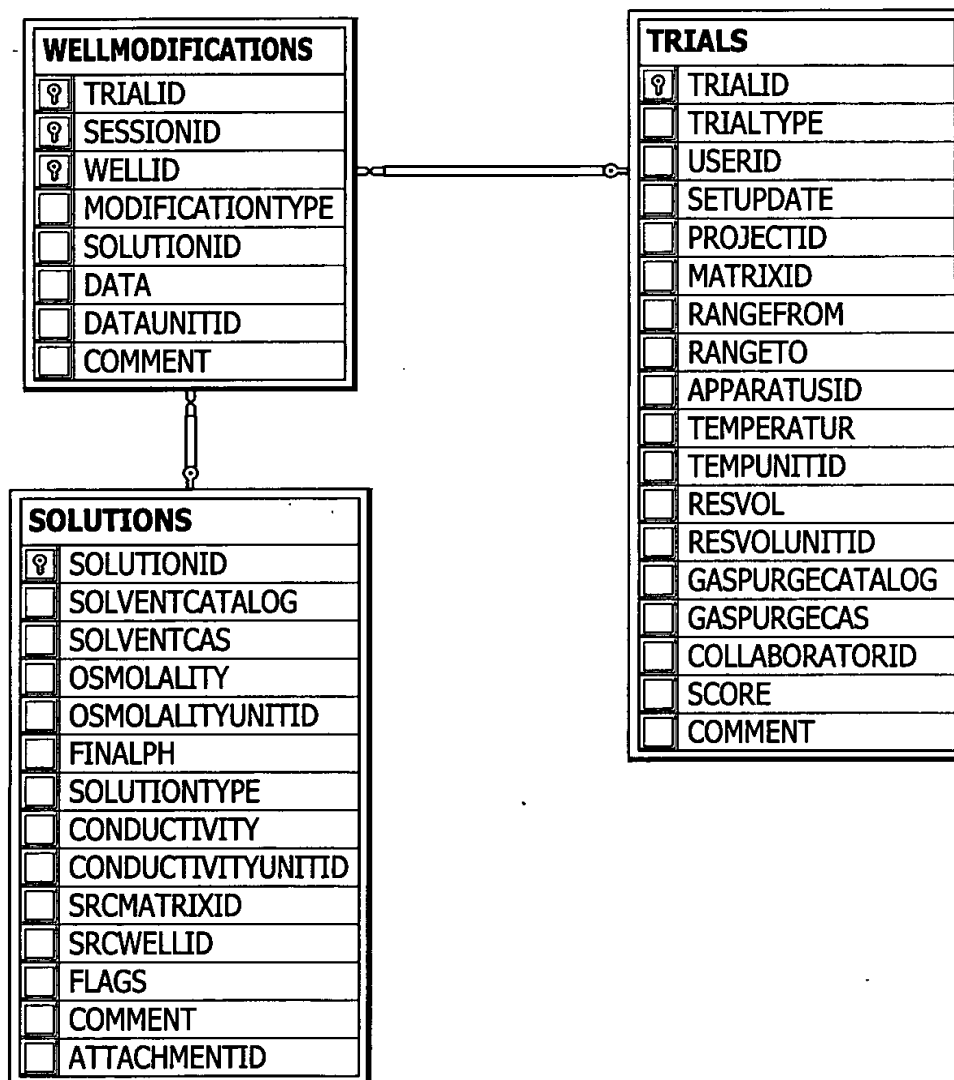
*Fig. 257*

*Fig. 258*

*Fig. 259*

*Fig. 260*

*Fig. 261*

*Fig. 262*

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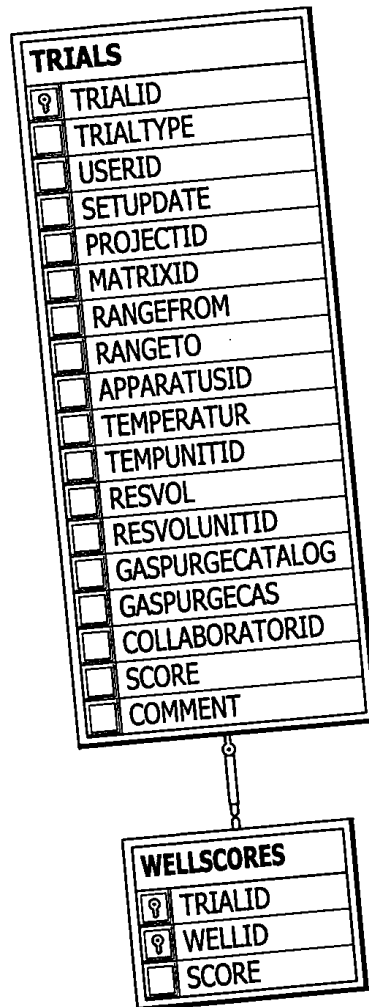


Fig. 263